A Homographic Best Approximation Problem with Application to Optimized Schwarz Waveform Relaxation

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Abstract

We present and study a homographic best approximation problem, which arises in the analysis of waveform relaxation algorithms with optimized transmission conditions. Its solution characterizes in each class of transmission conditions the one with the best performance of the associated waveform relaxation algorithm. We present the particular class of first order transmission conditions in detail and show that the new waveform relaxation algorithms are well posed and converge much faster than the classical one: the number of iterations to reach a certain accuracy can be orders of magnitudes smaller. We illustrate our analysis with numerical experiments.

Classification Codes 65M12, 65M55, 30E10.

Keywords Schwarz Method. Domain Decomposition. Best Approximation.

1 Introduction

Over the last decade, a new domain decomposition method for evolution problems has been developed, the so called Schwarz waveform relaxation method, see [7, 15, 17, 16, 18] for linear problems, and [8, 14] for nonlinear ones. The new method is well suited for solving evolution problems in parallel in space-time, and it permits not only local adaptation in space, but also in time. A significant drawback of this new method is its slow convergence on long time intervals. This problem can however be remedied by more effective transmission conditions, see [12, 6, 13, 9, 10, 22]. These transmission conditions are of differential type in both time and space, and depend on coefficients which are determined by optimization of the convergence factor. The associated best approximation problem has been studied for the optimized Schwarz waveform relaxation algorithm with Robin transmission conditions applied to the one-dimensional advection-diffusion equation in [11]. In higher dimensions, and for higher order transmission conditions, only numerical procedures have been used so far to solve the associated best approximation problem, see [22, 6]. We study here this best approximation problem in a more general setting: we search for a given function $f : \mathbb{C} \to \mathbb{C}$ the polynomial $s_n^*(z)$ of degree less than or equal to n, which minimizes over all s of degree less than or equal to n the quantity

$$\sup_{z \in K} \left| \frac{s(z) - f(z)}{s(z) + f(z)} e^{-lf(z)} \right|, \tag{1.1}$$

where K is a compact set in $\mathbb{C}$, and l is a non-negative real parameter.

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a compact interval and a class of functions defined on the same interval, find an element in the class which realizes the distance of the function to the class. If the class is the linear space of polynomials of degree less than or equal to n, and the distance is measured in the L^∞ norm, then the approximation problem is called a Chebyshev best approximation problem. This problem was studied in depth by Chebyshev and De la Vallée Poussin [23]. Its solution is characterized by an equioscillation property, and can be computed using the Remes algorithm [25, 24]. Later extensions concern rational approximations [5], and functions of a complex variable [28]. In the latter problem, Rivlin and Shapiro obtained equioscillation properties, from which they deduced uniqueness. In all cases existence is a matter of compactness. Problem (1.1) generalizes the complex best approximation problem by polynomials in two directions: first the difference $f-s$ is replaced by a homographic function in f and s, and second there is an exponential weight which involves the function f itself.

Our paper is organized as follows: in Section 2, we study the best approximation problem (1.1) and characterize its solutions. In Section 3, we present our model problem, an advection reaction diffusion equation, and introduce waveform relaxation algorithms for its space-time parallel solution. In Section 4, we use the results obtained for the homographic best approximation problem in Section 2 to optimize a particular class of Schwarz waveform relaxation algorithms for our model problem in one dimension, and then generalize the results to arbitrary spatial dimensions. We then show in Section 5 that the optimized algorithms from Section 4 are well posed and convergent in appropriate Sobolev spaces. Section 6 contains numerical results for the classical and optimized Schwarz waveform relaxation algorithms, which show how drastically the convergence behavior is improved in the optimized variants. We present our conclusions in Section 7.

2 A General Best Approximation Result

Let K be a closed set in $\mathbb{C}$, containing at least $n+2$ points. Let $f: K \to \mathbb{C}$ be a continuous function, such that for every z in K, $\Re f(z) > 0$. We denote by $\mathbf{P}_n$ the complex vector space of polynomials of degree less than or equal to n. We define

$$\delta_n(l) = \inf_{s\in\mathbf{P}_n} \sup_{z\in K} \left| \frac{s(z)-f(z)}{s(z)+f(z)} e^{-lf(z)} \right|, \tag{2.1}$$

and search for s_n^* in $\mathbf{P}_n$ such that

$$\sup_{z\in K} \left| \frac{s_n^*(z)-f(z)}{s_n^*(z)+f(z)} e^{-lf(z)} \right| = \delta_n(l). \tag{2.2}$$

2.1 Analysis of the Case $l = 0$ and K compact

We denote for simplicity by δ_n the number $\delta_n(0)$. Our analysis of (2.2) has three major steps: we first prove existence of a solution, then show that the solution must satisfy an equioscillation property, and finally, using the equioscillation property, we prove uniqueness of the solution. We define for any z_0 in $\mathbb{C}^* = \mathbb{C}\setminus 0$ and strictly positive δ the sets

$$\mathcal{C}(z_0,\delta) = \{z\in\mathbb{C}, \left|\frac{z-z_0}{z+z_0}\right| = \delta\},\ \mathcal{D}(z_0,\delta) = \{z\in\mathbb{C}, \left|\frac{z-z_0}{z+z_0}\right| < \delta\},\ \bar{\mathcal{D}}(z_0,\delta) = \mathcal{C}(z_0,\delta)\cup\mathcal{D}(z_0,\delta). \tag{2.3}$$

The following geometrical lemma is straightforward, see [1]:

Lemma 2.1 *For any δ different from 0 and 1, for any z_0 in $\mathbb{C}^* = \mathbb{C}\setminus 0$, the set $\mathcal{C}(z_0,\delta)$ in (2.3) is a circle with center at $\frac{1+\delta^2}{1-\delta^2}z_0$ and radius $\frac{2\delta}{|1-\delta^2|}|z_0|$. If $\delta < 1$, the set $\mathcal{D}(z_0,\delta)$ is the interior of the circle, and the exterior otherwise. The set $\mathcal{C}(z_0,1)$ is a line orthogonal to the line $(0,z_0)$.*

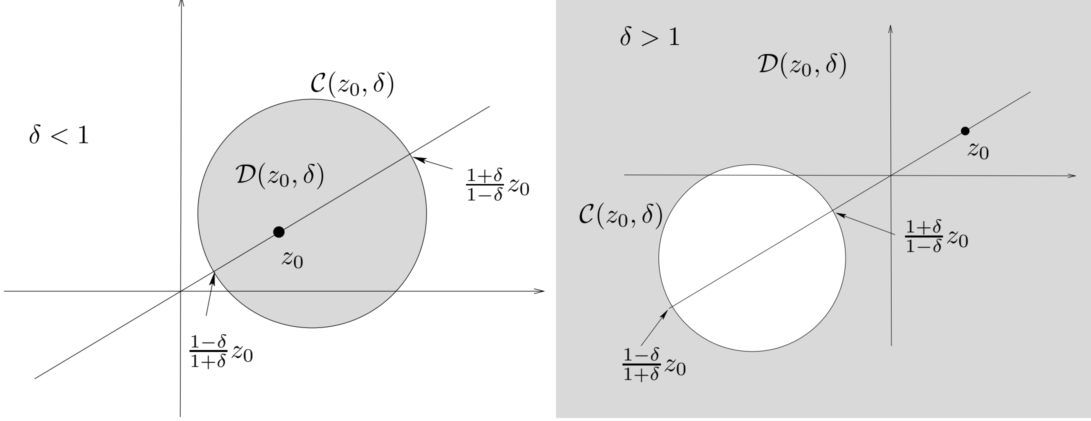

Figure 1: Illustration of the geometric Lemma 2.1: definition of $\mathcal{D}(z_0, \delta)$ in grey.

Theorem 2.1 (Existence) *For every $n \geq 0$, the number δ_n is strictly smaller than 1, and there exists at least one solution to problem (2.2) for $l = 0$.*

Proof Since $1 \in \mathbf{P}_n$, we have $\delta_n \leq \left\| \frac{1-f}{1+f} \right\|_\infty$. Now for any z in K, $\Re f(z) > 0$, and therefore $\left| \frac{1-f(z)}{1+f(z)} \right| < 1$. Since K is a compact set, we have $\delta_n < 1$. To prove existence, we take a minimizing sequence $\left(s_n^k\right)_{k \in \mathbb{N}}$ in $\mathbf{P}_n$, such that

$$\lim_{k \to \infty} \left\| \frac{s_n^k - f}{s_n^k + f} \right\|_\infty = \delta_n.$$

There exists a k_0 such that, for $k \geq k_0$, we have $\left\| \frac{s_n^k - f}{s_n^k + f} \right\|_\infty \leq C < 1$ with $C = (1 + \delta_n)/2$, and therefore by Lemma 2.1, $\frac{s_n^k}{f}(z)$ lies inside the disk $\bar{\mathcal{D}}(1, C)$, $C < 1$, for all z in K. Hence s_n^k is a bounded sequence in the finite dimensional space $\mathbf{P}_n$ and thus there exists a subsequence which converges to some s_n^* in $\mathbf{P}_n$, which attains the infimum. ■

We now investigate the equioscillation property of the solutions to (2.2). To do so, we need two further lemmas.

Lemma 2.2 *For a given vector $\boldsymbol{w} = (w_1, \ldots, w_m)$, $m \leq n+1$, such that w_j is in K for every j, let $U_{\boldsymbol{w}}$ be the open set in $\mathbf{P}_n$ of polynomials s such that $s(w_i) + f(w_i) \neq 0$ for all $i = 1, 2, \ldots, m$. If $w_i \neq w_j$ for $i \neq j$, the mapping*

$$\mathcal{A}_{\boldsymbol{w}} : U_{\boldsymbol{w}} \to \mathbb{C}^m, \quad s \mapsto \left(\frac{s(w_i) - f(w_i)}{s(w_i) + f(w_i)} \right)_{1 \leq i \leq m}$$

is a submersion: for any s in $U_{\boldsymbol{w}}$, the derivative $\mathcal{A}'_{\boldsymbol{w}}(s)$ is onto. Furthermore, its derivative is continuous with respect to s and w.

Proof The derivative of the mapping $A_{\boldsymbol{w}}$ is given by

$$\mathcal{A}'_{\boldsymbol{w}}(s) \cdot \tilde{s} = \left(\frac{2\tilde{s}(w_i) f(w_i)}{(s(w_i) + f(w_i))^2} \right)_{1 \leq i \leq m}, \quad \forall \tilde{s} \in \mathbf{P}_n. \tag{2.4}$$

Now for any $\boldsymbol{z}$ in $\mathbb{C}^m$, there exists a unique polynomial $\tilde{s}$ in $\mathbf{P}_{m-1}$, namely the Lagrange interpolation polynomial, such that

$$\forall i, 1 \leq i \leq m, \; \tilde{s}(w_i) = \frac{(s(w_i) + f(w_i))^2}{2f(w_i)} z_i,$$

and since $m - 1 \leq n$, $\tilde{s}$ is in $\mathbf{P}_n$ and $\mathcal{A}'_{\boldsymbol{w}}(s) \cdot \tilde{s} = \boldsymbol{z}$. The continuity of $\mathcal{A}'_{\boldsymbol{w}}$ with respect to s and $\boldsymbol{w}$ follows directly from (2.4). ■

Lemma 2.3 *Let s_n^* be a solution of (2.2) for $l = 0$. Let $\boldsymbol{z} = (z_1, \ldots, z_m)$ be a vector of m distinct points in K, $m \leq n+1$. We have:*

2. *let s be such that $\mathcal{A}'_{\boldsymbol{z}}(s_n^*)\ s = -\mathcal{A}_{\boldsymbol{z}}(s_n^*)$. Then for any ϵ, $0<\epsilon<1$, there exist positive $(\epsilon_1,\dots,\epsilon_m)$, and $t_0 \in (0,1)$, such that for any $t \in [\epsilon t_0, t_0]$ and for any z in K with $|z-z_i|<\epsilon_i$ for some i,*

$$\left|\frac{s_n^*(z)+ts(z)-f(z)}{s_n^*(z)+ts(z)+f(z)}\right| \le (1-\epsilon\frac{t_0}{2})\delta_n.$$

Proof

1. s_n^* is in $U_{\boldsymbol{z}}$ since otherwise δ_n would be infinite.

2. There exist strictly positive numbers $t'_0, \epsilon'_1, \dots, \epsilon'_m$ such that, for any t in $[0,t'_0]$, and any $\boldsymbol{w} = (w_1, w_2, \dots, w_m)$ with $w_j \in K$ and $|w_j - z_j| < \epsilon_j$ for all j, $s_n^* + ts$ is in $U_{\boldsymbol{w}}$. We now define $f_i(t,\boldsymbol{w}) = (\mathcal{A}_{\boldsymbol{w}}(s_n^*+ts))_i$, and we apply to f_i the first order Taylor-Lagrange formula in the first variable, about $t=0$. There exists τ_i in $(0,t)$ such that

$$f_i(t,\boldsymbol{w}) = f_i(0,\boldsymbol{w}) + t\partial_1 f_i(\tau_i,\boldsymbol{w}),$$

and by adding and subtracting $t\partial_1 f_i(0,\boldsymbol{z})$, we obtain

$$f_i(t,\boldsymbol{w}) = f_i(0,\boldsymbol{w}) + t\partial_1 f_i(0,\boldsymbol{z}) + t(\partial_1 f_i(\tau_i,\boldsymbol{w}) - \partial_1 f_i(0,\boldsymbol{z})).$$

Using now that s satisfies the equation $\mathcal{A}'_{\boldsymbol{z}}(s_n^*)s = -\mathcal{A}_{\boldsymbol{z}}(s_n^*)$, which reads componentwise $\partial_1 f_i(0,\boldsymbol{z}) = -f_i(0,\boldsymbol{z})$, we get

$$\begin{aligned} f_i(t,\boldsymbol{w}) &= f_i(0,\boldsymbol{w}) - tf_i(0,\boldsymbol{z}) + t(\partial_1 f_i(\tau_i,\boldsymbol{w}) - \partial_1 f_i(0,\boldsymbol{z})) \\ &= (1-t)f_i(0,\boldsymbol{w}) + t(f_i(0,\boldsymbol{w}) - f_i(0,\boldsymbol{z})) + t(\partial_1 f_i(\tau_i,\boldsymbol{w}) - \partial_1 f_i(0,\boldsymbol{z})). \end{aligned}$$

Since the functions f_i and $\partial_1 f_i$ are continuous in a neighbourhood of $(0,\boldsymbol{z})$, we obtain

$$f_i(t,\boldsymbol{w}) = (1-t)f_i(0,\boldsymbol{w}) + t\eta_i(\boldsymbol{w},\boldsymbol{w}-\boldsymbol{z}),$$

with some function $\eta_i(\boldsymbol{w},\boldsymbol{w}-\boldsymbol{z})$ continuous in $\boldsymbol{w}$, which tends to zero with $\boldsymbol{w}-\boldsymbol{z}$. Thus, for any positive ϵ, there exist positive $\epsilon_1,\dots,\epsilon_m$, and $0<t_0<1$, such that for any t in $[0,t_0]$ and any $\boldsymbol{w} = (w_1,\dots,w_m)$ with $|w_i - z_i| < \epsilon_i$ for all i,

$$\left|\frac{s_n^*(w_i)+ts(w_i)-f(w_i)}{s_n^*(w_i)+ts(w_i)+f(w_i)}\right| \le (1-t)\delta_n + \epsilon\delta_n\frac{t_0}{2} = (1-t+\epsilon\frac{t_0}{2})\delta_n.$$

Thus for t in $[\epsilon t_0, t_0]$ the result follows.

■

Theorem 2.2 (Equioscillation) *With the same assumptions as in Theorem 2.1, if the polynomial s_n^*, $n \ge 0$ is a solution of (2.2) for $l=0$, then there exist at least $n+2$ points $z_1,\cdots,z_{n+2}$ in K such that*

$$\left|\frac{s_n^*(z_i)-f(z_i)}{s_n^*(z_i)+f(z_i)}\right| = \left\|\frac{s_n^*-f}{s_n^*+f}\right\|_\infty. \tag{2.5}$$

Proof Let $z_1,\cdots,z_m$ be all distinct points of equioscillation, *i.e* satisfying (2.5). We know that $m \ge 1$, since we maximize over a compact set. Now suppose that $m \le n+1$ to reach a contradiction. First, we have $f(z_i) \ne 0$, since otherwise $\delta_n = 1$, which contradicts the result $\delta_n < 1$ from Theorem 2.1. We now use Lemma 2.3: we denote by $\mathcal{D}_i$ the disc with center z_i and radius ϵ_i defined in the lemma. By compactness, we have

$$\sup_{z\in K-(\cup\mathcal{D}_i)\cap K}\left|\frac{s_n^*(z)-f(z)}{s_n^*(z)+f(z)}\right| < \delta_n.$$

Then there exists a neighbourhood U of s_n^* such that for any s in U

$$\sup_{z\in K-(\cup\mathcal{D}_i)\cap K}\left|\frac{s(z)-f(z)}{s(z)+f(z)}\right| < \delta_n,$$

$$\sup_{z\in K}\left|\frac{s(z)-f(z)}{s(z)+f(z)}\right| = \sup_{z\in(\cup\mathcal{D}_i)\cap K}\left|\frac{s(z)-f(z)}{s(z)+f(z)}\right|.$$

For sufficiently small ϵ, by Lemma 2.3 there exists $t\in[\epsilon t_0, t_0]$ such that s_n^*+ts is in U, and we have

$$\left\|\frac{s_n^*+ts-f}{s_n^*+ts+f}\right\|_\infty < \delta_n,$$

which is a contradiction, since we found a polynomial s_n^*+ts which is a better approximation than s_n^* to f. ∎

Theorem 2.3 (Uniqueness) *With the same assumptions as in Theorem 2.1, the solution s_n^* of (2.2) for $l=0$ is unique for all $n\geq 0$.*

Proof We first show that the set of best approximations is convex: let s_n^* and $\tilde{s}_n^*$ be two polynomials of best approximation, θ a real number between 0 and 1, and let $s=\theta s_n^*+(1-\theta)\tilde{s}_n^*$. Then for any z in K, $\frac{s_n^*}{f}(z)$ and $\frac{\tilde{s}_n^*}{f}(z)$ are contained in $\bar{\mathcal{D}}(1,\delta_n)$, which is a disc since $\delta_n<1$, and hence convex. Thus for any z in K, $\frac{s}{f}(z)$ is also in $\bar{\mathcal{D}}(1,\delta_n)$, which means that $\left\|\frac{s-f}{s+f}\right\|_\infty\leq\delta_n$. Since δ_n is the infimum over all polynomials of degree n, we must have $\left\|\frac{s-f}{s+f}\right\|_\infty=\delta_n$ and s is therefore also a polynomial of best approximation. Therefore the set of best approximations is convex. Now we choose $n+2$ points $z_1,\ldots,z_{n+2}$ among the points of equioscillation of s. By definition $\frac{s}{f}(z_j)$ is on the boundary $\mathcal{C}(1,\delta_n)$ for all $j=1,2,\ldots,n+2$. But at the same time, $\frac{s_n^*}{f}(z_j)$ and $\frac{\tilde{s}_n^*}{f}(z_j)$ are in $\bar{\mathcal{D}}(1,\delta_n)$. The set $\bar{\mathcal{D}}(1,\delta_n)$ is however strictly convex, and thus a barycenter of two points can only be on the boundary, if the points coincide,

$$\frac{s_n^*(z_j)}{f(z_j)}=\frac{\tilde{s}_n^*(z_j)}{f(z_j)}=\frac{s(z_j)}{f(z_j)},\quad j=1,2,\ldots,n+2.$$

The difference $s_n^*-\tilde{s}_n^*$ therefore has at least $n+2$ roots, and since the polynomials are of degree at most n, they must coincide. ∎

We next study local best approximations. We define a map on $\mathbf{P}_n$ by

$$h(s)=\left\|\frac{s-f}{s+f}\right\|_\infty,\quad s\in\mathbf{P}_n,$$

and we search for local minima of h.

Theorem 2.4 (Local Minima) *Let s^* be a strict local minimum for h. Then s^* is the global minimum of h on $\mathbf{P}_n$.*

Proof We introduce a family of closed subsets of $\mathbf{P}_n$ for any $\delta>0$ by

$$\widetilde{\mathcal{D}}_\delta=\{s\in\mathbf{P}_n, h(s)\leq\delta\}.$$

These sets fulfills several properties:

(i) For any $\delta<1$, $\widetilde{\mathcal{D}}_\delta$ is a convex set. To see this, let s and $\tilde{s}$ be in $\widetilde{\mathcal{D}}_\delta$, and θ in $[0,1]$. For any z in K, $\frac{s}{f}(z)$ and $\frac{\tilde{s}}{f}(z)$ are in $\mathcal{D}(1,\delta)$ which is convex by Lemma 2.1. Hence $\theta\frac{s}{f}(z)+(1-\theta)\frac{\tilde{s}}{f}(z)$ is in $\mathcal{D}(1,\delta)$, which implies that $\theta\frac{s}{f}+(1-\theta)\frac{\tilde{s}}{f}$ is in $\widetilde{\mathcal{D}}_\delta$.

(ii) The map $\delta\mapsto\widetilde{\mathcal{D}}_\delta$ is increasing, as one can infer directly from its definition.

We now conclude the proof of the theorem: let (s^*,δ^*) be a strict local minimum for h, and (s^{**},δ^{**}) be another local minimum, with $\delta^*\geq\delta^{**}$, and $s^*\neq s^{**}$. Then there exists a convex neighbourhood U of s^*, such that for any s in U different from s^*, $h(s)>\delta^*$. Since $s^{**}\in\widetilde{\mathcal{D}}_{\delta^{**}}\subset\widetilde{\mathcal{D}}_{\delta^*}$, by the convexity of $\widetilde{\mathcal{D}}_{\delta^*}$, we have $[s^*,s^{**}]\subset\widetilde{\mathcal{D}}_{\delta^*}$. For ϵ small enough, we thus have $s_\epsilon=s^*+\epsilon(s^{**}-s^*)$ in $\widetilde{\mathcal{D}}_{\delta^*}$ and at the same time in U. This implies that $h(s_\epsilon)\leq\delta^*$ and at the same time $h(s_\epsilon)>\delta^*$, which is a contradiction. ∎

We now consider the best approximation problem (2.2) with a parameter $l > 0$.

Theorem 2.5 (Existence) *Let K be a closed set in $\mathbb{C}$, containing at least $n+2$ points. Let $f : K \to \mathbb{C}$ be a continuous function such that for every z in K, $\Re f(z) > 0$ and*

$$\Re f(z) \longrightarrow +\infty \text{ as } z \longrightarrow \infty \text{ in } K. \tag{2.6}$$

Then $\delta_n(l) < 1$ for all $n \geq 0$, and for l small enough, there exists a polynomial s_n^* solution to (2.2).

Proof By a standard compactness argument, property (2.6) implies that there exists $\alpha > 0$, such that for all $z \in K$, we have $\Re f(z) \geq \alpha > 0$. Now, $\left|\frac{1-f(z)}{1+f(z)} e^{-lf(z)}\right| \leq \left|\frac{1-f(z)}{1+f(z)}\right| e^{-l\alpha}$, and since $\Re f(z) > 0$, we have $\left|\frac{1-f(z)}{1+f(z)}\right| < 1$. Furthermore $1 \in \mathbf{P}_n$ for all $n \geq 0$, which implies that

$$\delta_n(l) \leq \left\| \frac{1-f}{1+f} e^{-lf} \right\|_\infty \leq e^{-l\alpha} < 1,$$

which proves the first part of the theorem.

For the second part, let $(s_n^k)_{k \in \mathbb{N}}$ be a minimizing sequence. Then for all ϵ, there exists a k_0, such that for all $k \geq k_0$ we have

$$\delta_n(l) \leq \left\| \frac{s_n^k - f}{s_n^k + f} e^{-lf} \right\|_\infty \leq \delta_n(l) + \epsilon, \tag{2.7}$$

and if we choose $\epsilon = \frac{1-\delta_n(l)}{2}$, we have

$$\left\| \frac{s_n^k - f}{s_n^k + f} e^{-lf} \right\|_\infty \leq \frac{1+\delta_n(l)}{2} < 1.$$

Let $\beta > \alpha$ and $K_\beta = K \cap \{z, \alpha \leq \Re f(z) \leq \beta\}$. By property (2.6), K_β is a compact set, and for β large enough, contains at least $n+2$ points. On this compact set, we obtain the estimate

$$\left\| \frac{s_n^k - f}{s_n^k + f} \right\|_{L^\infty(K_\beta)} = \left\| \frac{s_n^k - f}{s_n^k + f} e^{-lf} e^{lf} \right\|_{L^\infty(K_\beta)} \leq \left\| \frac{s_n^k - f}{s_n^k + f} e^{-lf} \right\|_{L^\infty(K_\beta)} e^{l\beta} \leq \frac{1+\delta_n(l)}{2} e^{l\beta},$$

and since $\frac{1+\delta_n(l)}{2} < 1$, if l is such that $\frac{1+\delta_n(l)}{2} e^{l\beta} < 1$, we get

$$\left\| \frac{s_n^k - f}{s_n^k + f} \right\|_{L^\infty(K_\beta)} < 1,$$

which shows that the numerical sequence $\|s_n^k\|_{L^\infty(K_\beta)}$ is bounded. Since K_β contains at least $n+2$ points , $\|\cdot\|_{L^\infty(K_\beta)}$ induces a norm on the finite dimensional vector space $\mathbf{P}_n$. Since on $\mathbf{P}_n$ all norms are equivalent, the minimizing sequence s_n^k is bounded in $\mathbf{P}_n$ for the norm $L^\infty(K)$. Hence s_n^k converges to a s_n^* in $L^\infty(K)$, which proves the existence by using (2.7). ■

The equioscillation property is shown like in the case $l = 0$: we first have the analogons of Lemmas 2.2 and 2.3 (the proofs are identical):

Lemma 2.4 *Let the assumptions of Theorem 2.5 be verified. Then for a given vector $\boldsymbol{w} = (w_1, \ldots, w_m)$, $m \leq n+1$, such that any w_i is in K and $w_i \neq w_j$ for $i \neq j$, the mapping*

$$\mathcal{A}_{\boldsymbol{w}} : U_{\boldsymbol{w}} \to \mathbb{C}^m, \quad s \mapsto \left(\frac{s(w_i) - f(w_i)}{s(w_i) + f(w_i)} e^{-lf(w_i)} \right)_{1 \leq i \leq m}$$

is a submersion. Furthermore its derivative is continuous with respect to s and w.

Lemma 2.5 *Let s_n^* be a solution of (2.2) for $l > 0$, and let $\boldsymbol{z} = (z_1, \ldots, z_m)$ be a vector of m distinct points in K, $m \leq n+1$. We have*

1. *s_n^* is in $U_{\boldsymbol{z}}$,*

and $t_0 \in]0,1[$, such that for any $t \in [\epsilon t_0, t_0]$ and for any z such that $|z - z_i| < \epsilon_i$ for some i,

$$\left|\frac{s_n^*(z) + t\tilde{s}(z) - f(z)}{s_n^*(z) + t\tilde{s}(z) + f(z)} e^{-lf(z)}\right| \le (1 - \epsilon\frac{t_0}{2})\delta_n.$$

Theorem 2.6 (Equioscillation) *With the assumptions of Theorem 2.5, if s_n^* is a solution of problem (2.2) for $l > 0$, then there exist at least $n+2$ points $z_1, \cdots, z_{n+2}$ in K such that*

$$\left|\frac{s_n^*(z_i) - f(z_i)}{s_n^*(z_i) + f(z_i)} e^{-lf(z_i)}\right| = \left\|\frac{s_n^* - f}{s_n^* + f} e^{-lf}\right\|_\infty.$$

Proof Using that

$$\delta_n(l) \le \left\|\frac{s_n^* - f}{s_n^* + f} e^{-lf}\right\|_\infty \le \delta_n e^{-l\inf_K \Re f} < 1,$$

the proof of the Theorem follows like in the case where $l = 0$. ■

To prove uniqueness in the general case, we need to assume compactness of K:

Theorem 2.7 (Uniqueness) *With the assumptions of Theorem 2.5, if K is a compact set, and l satisfies*

$$\delta_n(l) e^{l\sup_{z\in K}\Re f(z)} < 1, \tag{2.8}$$

then problem (2.2) has a unique solution s_n^* for all $n \ge 0$.

Proof We first prove that the set of best approximations is convex: let s_n^* and $\tilde{s}_n^*$ be two polynomials of best approximation, θ in $[0,1]$ and let $s = \theta s_n^* + (1-\theta)\tilde{s}_n^*$. For any z in D, $\frac{s_n^*}{f}(z)$ and $\frac{\tilde{s}_n^*}{f}(z)$ are in $\bar{\mathcal{D}}(1, \delta_n(l)e^{l\Re f(z)})$, which is convex since

$$\delta_n e^{l\Re f(z)} \le \delta_n e^{l\sup_K \Re f(z)} < 1$$

by condition (2.8). Thus for any z in K, $\frac{s}{f}(z)$ is in $\bar{\mathcal{D}}(1, \delta_n(l)e^{l\Re f(z)})$, which means that $\left\|\frac{s-f}{s+f}e^{-lf}\right\|_\infty \le \delta_n(l)$. Since $\delta_n(l)$ is the infimum, we have $\left\|\frac{s-f}{s+f}e^{-lf}\right\|_\infty = \delta_n(l)$ and s is also a best approximation. The conclusion follows now as in the proof of Theorem 2.3. ■

2.3 The Symmetric Case

We derive now specific results for the best approximation problems we are interested in in the context of waveform relaxation methods:

Definition 2.1 *The symmetric case of the homographic best approximation problem (2.2) satisfies*

$$\begin{cases} K \text{ is a closed set, symmetric with respect to the real axis, containing at least } n+2 \text{ points,} \\ \text{and for any } z \text{ in } K,\ f(\bar{z}) = \overline{f(z)}\ . \end{cases} \tag{2.9}$$

Theorem 2.8 *In the symmetric case* (2.9)*, if K is a compact set, if l is zero or is sufficiently small to satisfy* (2.8)*, then the polynomial of best approximation s_n^* of f in K has real coefficients.*

Proof If s_n^* is the polynomial of best approximation for f, we have

$$\sup_K \left|\frac{s_n^*(z)-f(z)}{s_n^*(z)+f(z)}e^{-lf(z)}\right| = \sup_K \left|\frac{s_n^*(\bar{z})-f(\bar{z})}{s_n^*(\bar{z})+f(\bar{z})}e^{-lf(\bar{z})}\right| = \sup_K \left|\frac{s_n^*(\bar{z})-\overline{f(z)}}{s_n^*(\bar{z})+\overline{f(z)}}e^{-l\overline{f(z)}}\right| = \sup_K \left|\frac{\overline{s_n^*(\bar{z})}-f(z)}{\overline{s_n^*(\bar{z})}+f(z)}e^{-lf(z)}\right|,$$

which shows that $\overline{s_n^*(\bar{z})} = s_n^*(z)$ for every z in K by uniqueness, and hence proves that s_n^* has real coefficients. ■

We denote by τ the complex involution $z \mapsto \bar{z}$. From now on, K_1 is a closed set in the upper half-plane $\Im z \ge 0$, and $K = K_1 \cup \tau(K_1)$. We consider the minimization problem restricted to the space $\mathbf{P}_n^r$ of polynomials with real coefficients on K_1, with the functional

$$h_l^r(s) = \left\|\frac{s-f}{s+f}e^{-lf}\right\|_{L^\infty(K_1)}, \tag{2.10}$$

$$\sup_{z\in K_1}\left|\frac{s_n^{r,*}(z)-f(z)}{s_n^{r,*}(z)+f(z)}e^{-lf(z)}\right| = \inf_{s\in\mathbf{P}_n^r}\sup_{z\in K_1}\left|\frac{s(z)-f(z)}{s(z)+f(z)}e^{-lf(z)}\right|. \tag{2.11}$$

Theorem 2.9 *In the symmetric case described in* (2.9)*, suppose that K_1 is compact, l is zero or is sufficiently small to satisfy* (2.8)*. Then any strict local minimum of h_l^r in $\mathbf{P}_n^r$ is a global minimum in $\mathbf{P}_n^r$, and is unique.*

Proof With condition (2.8), the proof is the same as in Theorem 2.4. ■

Corollary 2.10 *Under the assumptions in Theorem 2.9, any strict local minimum of h_l^r in $\mathbf{P}_n^r$ is the global minimum for the complex best approximation problem* (2.2)*.*

Proof By Theorem 2.8, the solution of the complex problem (2.2) is real, and therefore is a global minimum for h_l^r. But if there is a strict local minimum for h_l^r, it is the only global minimum of h_l^r, and therefore coincides with the solution of the complex problem (2.2). ■

In the non compact case, there is no such result available, but we will only need to solve a particular problem. We introduce the notations $\mathbf{P}_1^+ = \{s = p + qz, p \geq 0, q \geq 0\}$ and $\mathbb{C}^+ = \{z, \Re z \geq 0, \Im z \geq 0\}$ and consider the problem of finding s_1^+ in $\mathbf{P}_1^+$ such that:

$$\sup_{z\in K_1}\left|\frac{s_1^{+,*}(z)-f(z)}{s_1^{+,*}(z)+f(z)}e^{-lf(z)}\right| = \inf_{s\in\mathbf{P}_1^+}\sup_{z\in K_1}\left|\frac{s(z)-f(z)}{s(z)+f(z)}e^{-lf(z)}\right|. \tag{2.12}$$

Theorem 2.11 *Suppose $K_1 \subset \mathbb{C}^+$, then any strict local minimum of h_l^r in $\mathbf{P}_1^+$ is a global minimum.*

Proof The proof is an extension of the proof of Theorem 2.4. We introduce a family of subsets of $\mathbf{P}_1^+$ for any $\delta > 0$ by

$$\widetilde{\mathcal{D}}_\delta^l = \{s \in \mathbf{P}_1^+, h^l(s) \leq \delta\}.$$

The only difference compared to the proof of Theorem 2.4 is the proof of property (i), which states that for any $\delta < 1$, $\widetilde{\mathcal{D}}_\delta^l$ is a convex set. To show this, let s and $\tilde{s}$ be in $\widetilde{\mathcal{D}}_\delta^l$. For any z in K_1, $s(z)$ and $\tilde{s}(z)$ are in $\mathcal{D}(f(z), \delta e^{l\Re f(z)}) \cap \mathbb{C}^+$. If $\delta e^{l\Re f(z)} < 1$, $\mathcal{D}(f(z), \delta e^{l\Re f(z)})$ is convex by Lemma 2.1, whereas if $\delta e^{l\Re f(z)} \geq 1$, since $f(z) \in \mathbb{C}^+$, $\mathbb{C}^+ \subset \mathcal{D}(f(z), \delta e^{l\Re f(z)})$, and $\mathbb{C}^+ \cap \mathcal{D}(f(z), \delta e^{l\Re f(z)}) = \mathbb{C}^+$. In any case $\mathcal{D}(f(z), \delta e^{l\Re f(z)}) \cap \mathbb{C}^+$ is convex. Then, for any z in K_1, such that $\Im z > 0$, we have $\frac{1}{2}(s(z) + \tilde{s}(z))$ is in $\mathcal{D}(f(z), \delta e^{l\Re f(z)}) \cap \mathbb{C}^+$. Thus $\frac{1}{2}(s + \tilde{s})$ is in $\widetilde{\mathcal{D}}_\delta^l$ which proves the convexity, since $\widetilde{\mathcal{D}}_\delta^l$ is a closed set. Having established convexity, the result follows as in Theorem 2.4. ■

Remark 2.1 *It is tempting at this stage to believe that the number of equioscillation points for the real problem* (2.11) *or* (2.12) *is also $\geq n + 2$. We will prove in Section 4 that this is true for our special problem, when $n = 1$ and the size of K_1 is sufficiently large in $\mathbb{C}^+$. However, it is not true in general, and we will show a counterexample at the end of Section 4.1.1.*

3 Model Problem and Schwarz Waveform Relaxation Algorithms

The homographic best approximation problem (2.1), (2.2) we studied in Section 2 is important for solving evolution problems in parallel. To define a parallel algorithm in space-time, Schwarz waveform relaxation algorithms use a decomposition of the spatial domain into subdomains, and then compute iteratively subdomain solutions in space-time, which like in the case of classical Schwarz methods are becoming better and better approximations to the entire solution, see [16]. Our guiding example here is the advection reaction diffusion equation in $\mathbb{R}^N$,

$$\partial_t u + (\boldsymbol{a} \cdot \boldsymbol{\nabla})u - \nu \Delta u + bu = f.$$

We consider here for the analysis only the decomposition into two half-spaces, since we improve the local coupling between neighboring subdomains. Our numerical experiments in Section 6 show however that coordinate $(x, \boldsymbol{y}) = (x, y_1, \cdots, y_{N-1})$, and use for the advection vector the notation $\boldsymbol{a} = (a, \boldsymbol{c})$, which leads to

$$\mathcal{L}u = \partial_t u + a\partial_x u + (\boldsymbol{c} \cdot \boldsymbol{\nabla}_{\boldsymbol{y}})u - \nu\Delta u + bu = f, \quad \text{in } \Omega \times (0, T). \tag{3.1}$$

The diffusion coefficient ν is strictly positive, and we assume that a and b are constants which do not both vanish simultaneously. The case of the heat equation needs special treatment and can be found in [9]. Without loss of generality, we can assume that the advection coefficient a in the x direction is non-negative, since $a < 0$ amounts to changing x into $-x$. We can also assume that the reaction coefficient b is non-negative. If not, a change of variables $v = ue^{-\zeta t}$, with $\zeta + b > 0$ will lead to (3.1) with a positive reaction coefficient. We split $\Omega = \mathbb{R}^N$ into two subdomains $\Omega_1 = (-\infty, L) \times \mathbb{R}^{N-1}$ and $\Omega_2 = (0, \infty) \times \mathbb{R}^{N-1}$, $L \geq 0$. A Schwarz waveform relaxation algorithm consists then of solving iteratively subproblems on $\Omega_1 \times (0, T)$ and $\Omega_2 \times (0, T)$ using general transmission conditions at the interfaces $\Gamma_0 = \{0\} \times \mathbb{R}^{N-1}$ and $\Gamma_L = \{L\} \times \mathbb{R}^{N-1}$, *i.e.* defining a sequence (u_1^k, u_2^k), for $k \in \mathbb{N}$, such that

$$\begin{array}{rclcrcl} \mathcal{L}u_1^k &=& f \quad \text{in } \Omega_1 \times (0,T), & \qquad & \mathcal{L}u_2^k &=& f \quad \text{in } \Omega_2 \times (0,T), \\ u_1^k(\cdot,\cdot,0) &=& u_0 \quad \text{in } \Omega_1, & & u_2^k(\cdot,\cdot,0) &=& u_0 \quad \text{in } \Omega_2, \\ \mathcal{B}_1 u_1^k &=& \mathcal{B}_1 u_2^{k-1} \text{ on } \Gamma_L \times (0,T), & & \mathcal{B}_2 u_2^k &=& \mathcal{B}_2 u_1^{k-1} \text{ on } \Gamma_0 \times (0,T), \end{array} \tag{3.2}$$

where $\mathcal{B}_1$ and $\mathcal{B}_2$ are linear operators in space and time, possibly pseudo-differential, and an initial guess $\mathcal{B}_2 u_1^0(0, \cdot, \cdot)$ and $\mathcal{B}_1 u_2^0(L, \cdot, \cdot)$, $t \in (0, T)$, needs to be provided.

The classical Schwarz waveform relaxation algorithm is obtained by choosing $\mathcal{B}_1$ and $\mathcal{B}_2$ equal to the identity, like in the case of the Schwarz domain decomposition methods for elliptic problems [27, 21]. With this choice, the algorithm is convergent only with overlap. This algorithm has been studied in [11] and [22] for the present model problem; for earlier studies, see [15, 17, 16]

A better choice, which leads to faster algorithms, which can be convergent even without overlap, is

$$\mathcal{B}_j = \partial_x + \mathcal{S}_j(\boldsymbol{\nabla}_{\boldsymbol{y}}, \partial_t), j = 1, 2, \tag{3.3}$$

where the $\mathcal{S}_j$ are ordinary linear pseudo differential operators in $(\boldsymbol{y}, t)$, related to their total symbols $\sigma_j(\boldsymbol{\eta}, \omega)$ by [19]

$$\mathcal{S}_j(\boldsymbol{\nabla}_{\boldsymbol{y}}, \partial_t)u(\boldsymbol{y}, t) = (2\pi)^{-n/2} \int \sigma_j(\boldsymbol{\eta}, \omega)\hat{u}(\boldsymbol{\eta}, \omega)e^{i(\boldsymbol{\eta} \cdot \boldsymbol{y} + \omega t)}\, d\boldsymbol{\eta}\, d\omega.$$

The best operators $\mathcal{S}_j$ are related to transparent boundary operators, which have first been exploited in [4] for stationary problems, and in [12] for time dependent problems. They can be found by the following analysis. Let e_i^k be the error in Ω_i, *i.e.* $e_i^k = u_i^k - u$. Using Fourier transform in time with parameter ω and in $\boldsymbol{y}$ with parameter $\boldsymbol{\eta}$, the Fourier transforms $\hat{e}_j^k$ in time and $\boldsymbol{y}$ of e_j^k are solution of the ordinary differential equation in the x variable

$$-\nu\frac{\partial^2 \hat{e}}{\partial x^2} + a\frac{\partial \hat{e}}{\partial x} + \big(i(\omega + \boldsymbol{c} \cdot \boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2 + b\big)\hat{e} = 0.$$

The characteristic roots are

$$r^+ = \frac{a + \sqrt{d}}{2\nu}, \quad r^- = \frac{a - \sqrt{d}}{2\nu}, \quad d = a^2 + 4\nu(i(\omega + \boldsymbol{c} \cdot \boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2 + b).$$

The complex square root in this text is always with strictly positive real part. In order to work with at least square integrable functions in time and space, we seek for solutions which do not increase exponentially in x. Since $\Re r^+ > 0$ and $\Re r^- < 0$, we obtain

$$\hat{e}_1^k(x, \boldsymbol{\eta}, \omega) = \alpha_1^k(\boldsymbol{\eta}, \omega)e^{r^+(x-L)}, \qquad \hat{e}_2^k(x, \boldsymbol{\eta}, \omega) = \alpha_2^k(\boldsymbol{\eta}, \omega)e^{r^- x}. \tag{3.4}$$

Inserting (3.4) into the transmission conditions (3.3), we find that for any $k \geq 2$,

$$\alpha_j^{k+1} = \rho\, \alpha_j^{k-1}, \quad j = 1, 2,$$

with the convergence factor

$$\rho = \frac{r^- + \sigma_1}{r^+ + \sigma_1} \cdot \frac{r^+ + \sigma_2}{r^- + \sigma_2}\, e^{(r^- - r^+)L}, \quad \forall \omega \in \mathbb{R},\ \boldsymbol{\eta} \in \mathbb{R}^{N-1}. \tag{3.5}$$

$$\sigma_1 = -r^-, \qquad \sigma_2 = -r^+, \tag{3.6}$$

then algorithm (3.2) converges in 2 steps, independently of the initial guess. This is an optimal result, since the solution on one subdomain necessarily depends on the right hand side function f on the other subdomain, and hence at least one communication is necessary for convergence. The choice in (3.6) however leads to non-local operators $\mathcal{S}_j$, since r^+ and r^- are not polynomials in the dual variables, and non-local operators are less convenient to implement and more costly to use than local ones. It is therefore of interest to approximate the optimal choice σ_j in (3.6) corresponding to the optimal transmission operators by polynomials in $(\omega, \boldsymbol{\eta})$, which leads to differential operators $\mathcal{S}_j$. We suppose in the sequel that the $\mathcal{S}_j$, $j = 1, 2$, are chosen in a symmetric way, *i.e.* their symbols are of the form

$$\sigma_1 = \frac{-a+s}{2\nu}, \quad \sigma_2 = \frac{-a-s}{2\nu},$$

where s is a polynomial in the dual variables. Defining the complex function z of $(\omega, \boldsymbol{\eta})$ by

$$z = 4\nu\big(i(\omega + \boldsymbol{c}\cdot\boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2\big), \tag{3.7}$$

we obtain for the convergence factor (3.5)

$$\rho(z,s) = \left(\frac{s(z) - \sqrt{a^2+4\nu b + z}}{s(z) + \sqrt{a^2+4\nu b+z}}\right)^2 e^{-\frac{L}{\nu}\sqrt{a^2+4\nu b+z}}. \tag{3.8}$$

In numerical computations, the frequencies ω and $\boldsymbol{\eta}$ are bounded, *i.e.* $|\omega| \le \omega_{max}$ and $|\eta_j| \le \eta_{j,max}$ where $\omega_{\max}$ is a discrete frequency which can be estimated by $\omega_{\max} = \pi/\Delta t$, where Δt is the time step, and similarly $\eta_{j,\max} = \pi/\Delta y_j$. In the nonoverlapping case, we define the compact set

$$K = \{z \in \mathbb{C}, |\omega| \le \omega_{max}, |\eta_j| \le \eta_{j,max}, j = 1, \cdots, n-1\}.$$

In the overlapping case,we shall also consider $\omega_{\max} = \infty$ and $\eta_{j,max} = \infty$, which leads to a non compact set K.

For any integer n we search for s_n^* in $\mathbf{P}_n$, the complex space of polynomials of degree less than or equal to n with complex coefficients, such that

$$\sup_{z\in K} |\rho(z, s_n^*)| = \inf_{s\in\mathbf{P}_n} \sup_{z\in K} |\rho(z,s)|. \tag{3.9}$$

Problem (3.9) is a special case of (2.2) with

$$f(z) = \sqrt{\xi_0^2 + z}, \quad l = \frac{L}{2\nu}, \quad \xi_0 = \sqrt{a^2+4\nu b}, \tag{3.10}$$

and the assumptions on f in Section 2 are verified with $\Re f(z) \ge \xi_0 > 0$.

We focus in the sequel on first order approximations, *i.e.* $s = p + qz$, which leads to first order optimized Schwarz waveform relaxation algorithms (3.2) with transmission conditions

$$\mathcal{S} = p + 4q\nu(\partial_t + (\boldsymbol{c}\cdot\boldsymbol{\nabla}_{\boldsymbol{y}}) - \nu\Delta_{\boldsymbol{y}}), \quad \mathcal{B}_1 = \partial_x - \frac{a}{2\nu} + \frac{1}{2\nu}\mathcal{S}, \quad \mathcal{B}_2 = \partial_x - \frac{a}{2\nu} - \frac{1}{2\nu}\mathcal{S}. \tag{3.11}$$

The case of zeroth order transmission conditions, $q = 0$, was studied in [11] for one dimensional problems, and existence and convergence proofs together with numerical experiments were shown in [22] for two dimensional problems. Using the general results from Section 2, we now solve the best approximation problem with first degree polynomials in one dimension.

4 Study and Optimization of the Convergence Factor

We start with the one-dimensional case, for which the conditions of Section 2.3 hold, with $K_1 = i[0, \omega_{max}]$. We proved in Theorem 2.8 that the polynomial of best approximation in the complex domain K has real coefficients, and we established in Corollary 2.10 the connection between the complex problem and the properties for the real problem, in both the overlapping and nonoverlapping cases, which allows us to compute the optimal choice for the coefficients p and q in the optimized Schwarz waveform relaxation algorithm (3.2) with transmission conditions (3.11).

If $p, q \in \mathbb{R}$, then the modulus of the convergence factor (3.8) is

$$R(\xi, p, q, \xi_0, L) = \frac{(\xi - p)^2 + (\xi^2 - \xi_0^2)(2q\xi - 1)^2}{(\xi + p)^2 + (\xi^2 - \xi_0^2)(2q\xi + 1)^2} e^{-\frac{L}{\nu}\xi}. \tag{4.1}$$

where we used the change of variables

$$\xi = \Re(\sqrt{a^2 + 4\nu(b + i\omega)}), \tag{4.2}$$

and $\xi_0 = \sqrt{a^2 + 4\nu b}$ from (3.10). We first propose and analyze a low frequency approximation for the first order transmission conditions, and then solve the best approximation problem, to derive optimized parameters p and q. In both cases, we analyze the performance of the overlapping ($L > 0$) and non-overlapping case ($L = 0$).

4.1 Low Frequency Approximation

As a simple approach, a low frequency approximation of the optimal transmission conditions (3.6) can be used to determine the two parameters p and q. We call this case T1 for Taylor of order one in the sequel. Using a Taylor expansion of the square root $\sqrt{a^2 + 4\nu(b + i\omega)}$ in (3.6) about $\omega = 0$, we find

$$\sqrt{a^2 + 4\nu(b + i\omega)} = \sqrt{a^2 + 4\nu b} + \frac{2\nu}{\sqrt{a^2 + 4\nu b}} i\omega + O(\omega^2),$$

and hence for the parameters p and q the values

$$p = p_T = \sqrt{a^2 + 4\nu b} \quad \text{and} \quad q = q_T = \frac{1}{2\sqrt{a^2 + 4\nu b}}. \tag{4.3}$$

4.1.1 The Non-Overlapping Case

For $L = 0$, $p = p_T$ and $q = q_T$, the convergence factor (4.1) becomes

$$R(\xi, p_T, q_T, \xi_0, 0) = \left(\frac{\xi - \xi_0}{\xi + \xi_0}\right)^2. \tag{4.4}$$

The bound on the frequency parameter ω given before, $|\omega| \leq \omega_{max} = \pi/\Delta t$, gives a bounded range $\xi_0 \leq \xi \leq \xi_{\max}$, where

$$\xi_{\max} = \sqrt{\frac{\sqrt{\xi_0^4 + 16\nu^2\omega_{\max}^2} + \xi_0^2}{2}}. \tag{4.5}$$

Proposition 4.1 (T1 Convergence Factor Estimate without Overlap) *The convergence factor in (4.4) is for $\xi_0 \leq \xi < \xi_{max}$ uniformly bounded by*

$$R_{T1}(\xi_0, \xi_{max}) = \left(\frac{\xi_{\max} - \xi_0}{\xi_{\max} + \xi_0}\right)^2. \tag{4.6}$$

For Δt small, this maximum can be expanded as $1 - 2\xi_0\sqrt{\frac{2}{\nu\pi}}\sqrt{\Delta t} + O(\Delta t)$.

Proof Since $R(\xi, p_T, q_T, \xi_0, 0)$ is a monotonically increasing function for $\xi \geq \xi_0$, the bound for $\xi_0 \leq \xi \leq \xi_{\max}$ is attained at $\xi = \xi_{\max}$, which leads, using the variable transform (4.2) and $\omega_{\max} = \frac{\pi}{\Delta t}$ to the bound given in (4.6). ■

Remark 4.1 *The convergence factor estimate (4.6) for the first order Taylor transmission conditions is the square of the convergence factor estimate found in [11] for the zeroth order Taylor transmission conditions.*

With $L > 0$, $p = p_T$ and $q = q_T$, and the change of variables (4.2), the convergence factor (4.1) becomes

$$R(\xi, p_T, q_T, \xi_0, L) = \left(\frac{\xi - \xi_0}{\xi + \xi_0}\right)^2 e^{-\frac{\xi L}{\nu}}. \tag{4.7}$$

We first present a convergence factor estimate for ω in $\mathbb{R}$.

Proposition 4.2 (T1 Convergence Factor Estimate with Overlap) *The convergence factor in (4.7) satisfies*

$$R_{T1}^{\infty}(\xi_0, L) = \max_{\xi_0 \le \xi < +\infty} R(\xi, p_T, q_T, \xi_0, L) = \left(\frac{\bar{\xi} - \xi_0}{\bar{\xi} + \xi_0}\right)^2 e^{-\frac{L\bar{\xi}}{\nu}}, \quad \text{with } \bar{\xi} = \sqrt{\xi_0^2 + \frac{4\nu\xi_0}{L}}. \tag{4.8}$$

For L small, this maximum can be expanded as $1 - 4\sqrt{\frac{\xi_0}{\nu}}\sqrt{L} + O(L)$.

Proof Taking a derivative of the convergence factor $R(\xi, p_T, q_T, \xi_0, L)$ defined in (4.7) with respect to ξ shows that there is a unique maximum for $\xi \ge \xi_0$ at $\xi = \bar{\xi}$ given in (4.8). Evaluating R for $\xi = \bar{\xi}$ and expanding for L small leads to the asymptotic result. ■

In a numerical computation, the overlap L is in general not a fixed quantity, one can only afford a few grid cells overlap, $L = C_1\Delta x$. In addition, there is also often a relation between the time and space step, of the form $\Delta t = C_2 \Delta x^{\beta}$, $\beta > 0$, due to accuracy or stability constraints. There exists a limiting value of the overlap, namely

$$L_1 = \frac{8\nu\xi_0}{\sqrt{\xi_0^4 + 16\nu\omega_{\max}} - \xi_0^2}, \tag{4.9}$$

such that for $L > L_1$, $\xi_{\max} > \bar{\xi}$, and hence the contraction factor in (4.8) is relevant. On the other hand, if $L \le L_1$, then $\xi_{\max} \le \bar{\xi}$ and hence numerically the contraction factor in (4.8) becomes irrelevant. Numerically, the relevant bound is therefore by monotonicity

$$R_{T1}(\xi_0, \xi_{\max}, L) = \max_{\xi_0 \le \xi \le \xi_{\max}} R(\xi, p_T, q_T, \xi_0, L) = \begin{cases} R_{T1}^{\infty}(\xi_0, L), & \text{if } L > L_1, \\ \left(\frac{\xi_{\max} - \xi_0}{\xi_{\max} + \xi_0}\right)^2 e^{-\frac{L\xi_{\max}}{\nu}}, & \text{if } L \le L_1. \end{cases} \tag{4.10}$$

Proposition 4.3 (T1 Discrete Convergence Factor Estimate with Overlap) *If $L = C_1\Delta x$ and $\Delta t = C_2\Delta x^{\beta}$, then the bound in (4.10) on the convergence factor has for Δx small the expansion*

$$R_{T1}(\xi_0, \xi_{\max}, L) = \begin{cases} 1 - 4\sqrt{\frac{C_1\xi_0}{\nu}}\sqrt{\Delta x} + O(\Delta x), & \text{if } \beta > 1, \text{ or } \beta = 1 \text{ and } \frac{C_1}{C_2} > \frac{2\xi_0}{\pi}, \\ 1 - \frac{\sqrt{2}(2C_2\xi_0 + C_1\pi)}{\sqrt{C_2\pi\nu}}\sqrt{\Delta x} + O(\Delta x), & \text{if } \beta = 1 \text{ and } \frac{C_1}{C_2} \le \frac{2\xi_0}{\pi}, \\ 1 - 2\xi_0\sqrt{\frac{2C_2}{\pi\nu}}\Delta x^{\frac{\beta}{2}} + o(\Delta x^{\frac{\beta}{2}}), & \text{if } 0 < \beta < 1. \end{cases} \tag{4.11}$$

Proof Expanding (4.9) for Δt small, we obtain

$$L_1 = \frac{2\xi_0}{\pi}\Delta t + O(\Delta t^2),$$

and comparing with $L = C_1\Delta x$, using that $\Delta t = C_2\Delta x^{\beta}$, we obtain the first case in (4.11). For the second case, one can set $\beta = 1$ and directly expand the second case of (4.10) to find the result given. For the last case, the expansion of the exponential term gives

$$e^{-\frac{L\xi_{\max}}{\nu}} = 1 - C_1\sqrt{\frac{2\pi}{C_2\nu}}\Delta x^{1-\frac{\beta}{2}} + O(\Delta x^{2-\beta}),$$

and the coefficient in front of the exponential in (4.10) has the expansion

$$\frac{\xi_{\max} - \xi_0}{\xi_{\max} + \xi_0} = 1 - \xi_0\sqrt{\frac{2C_2}{\pi\nu}}\Delta x^{\frac{\beta}{2}} + O(\Delta x^{\beta}).$$

Hence the result follows. ■

We now use the general results from Section 2 on the homographic best approximation problem to optimize the waveform relaxation algorithm with transmission conditions (3.11) for the overlapping and non-overlapping case. We call this case O1 for optimized of order one in the sequel.

4.2.1 The Non-Overlapping Case

The domain of definition for $f(z) = \sqrt{\xi_0^2 + 4\nu z}$ with $z = i\omega$ is $K = i[0, \omega_{max}] \cup -i[0, \omega_{max}]$. By Theorems 2.1 and 2.3, the problem (3.9) in $\mathbf{P}_1$ has a unique solution $s_1^* = p^* + 4\nu i\omega q^*$. By Theorem 2.8, s_1^* has real coefficients. Therefore, (p^*, q^*) is the unique pair of real numbers such that

$$\inf_{p,q\in\mathbb{R}} \sup_{\xi_0\leq\xi\leq\xi_{\max}} R(\xi, p, q, \xi_0, 0) = \sup_{\xi_0\leq\xi\leq\xi_{\max}} R(\xi, p^*, q^*, \xi_0, 0), \tag{4.12}$$

and we denote by R_{O1} the maximum of the convergence factor,

$$R_{O1}(\xi_0, \xi_{max}) = \sup_{\xi_0\leq\xi\leq\xi_{\max}} R(\xi, p^*, q^*, \xi_0, 0).$$

$R_{O1}(\xi_0, \xi_{max})$ is equal to δ_1^2 with the notation from Section 2.

Lemma 4.1 *The solution (p^*, q^*) of the min-max problem (4.12) satisfies $p^* > 0$ and $q^* \geq 0$.*

Proof Knowing from Theorem 2.1 that $\delta_1 < 1$, and taking $\xi = \xi_0$ in (4.1), we first see that $p^* > 0$. Now for positive p and q, we see in (4.1) that $R(\xi, p, q, \xi_0, 0) \leq R(\xi, p, -q, \xi_0, 0)$, which proves that $q^* \geq 0$. ∎
Because of the symmetry of the domain K, $\left\|\frac{s_1^*-f}{s_1^*+f}\right\|$ equioscillates at least twice in $[0, \omega_{max}]$. We show now that for sufficiently large ω_{max}, the solution actually equioscillates three times on $[0, \omega_{max}]$, and we give implicit formulas for the solution p^* and q^*.

Theorem 4.1 (O1 Convergence Factor Estimate without Overlap) *For $\xi_{\max}$ sufficiently large, the solution of (4.12) equioscillates three times, i.e. p^* and q^* are the unique solution of the system of equations*

$$R(\xi_0, p, q, \xi_0, 0) = R(\bar{\xi}(p, q), p, q, \xi_0, 0) = R(\xi_{\max}, p, q, \xi_0, 0) \tag{4.13}$$

where $\bar{\xi}(p, q)$ is the second of the three distinct ordered positive roots (for $p > (1 + \sqrt{2})\xi_0$) of the bi-cubic polynomial

$$\begin{aligned} P(\xi) \quad = \quad & 32q^3\xi^6 - 16q(-3qp + 4q^2\xi_0^2 + 1)\xi^4 \\ & +(8q\xi_0^2 + 32q^3\xi_0^4 - 24qp^2 - 16q^2\xi_0^2 p + 8p)\xi^2 - 4(\xi_0 - p)(\xi_0 + p)(2q\xi_0^2 - p). \end{aligned} \tag{4.14}$$

The optimal parameters and the bound on the convergence factor, which is the common value $R_{O1}(\xi, \xi_0, \xi_{max})$ in (4.13) *at point $(p, q) = (p^*, q^*)$, have the expansions*

$$p^* \sim \xi_0^{\frac{3}{4}} \xi_{\max}^{\frac{1}{4}}, \quad \hat{q}^* \sim \frac{1}{2\xi_0^{\frac{1}{4}}} \xi_{\max}^{-\frac{3}{4}}, \quad R_{O1}(\xi_0, \xi_{max}) \sim 1 - 4\xi_0^{\frac{1}{4}} \xi_{\max}^{-\frac{1}{4}}. \tag{4.15}$$

Proof We start this proof by studying the variation of R for fixed p and q: the polynomial P given in (4.14) is the numerator of the partial derivative of R with respect to ξ. Therefore its roots determine the extrema of R. Since P is a bi-cubic polynomial with real coefficients, it has one, two or three positive distinct real roots. In the first two cases, since $R(0, p, q, \xi_0, 0) = 1$, $R \leq 1$ for $\xi \geq \xi_0$ and $R \longrightarrow 1$ as $\xi \longrightarrow \infty$, R reaches a unique minimum in $[\xi_0, \xi_{max}]$, and therefore if $p = p^*$ and $q = q^*$, R equioscillates at points ξ_0 and ξ_{max} only. If there are three ordered distinct positive real roots, then the second one, $\bar{\xi}$, must correspond to a maximum of R and the other ones to minima. The maximum of R can thus be attained at the local maximum at $\bar{\xi}$, or at the end-points ξ_0 and $\xi_{\max}$.

We now focus on the condition for these three points to give equioscillations for R, *i.e.* on solving (4.13). We first prove that the equation $R(\xi_0, p, q, \xi_0, 0) = R(\xi_{\max}, p, q, \xi_0, 0)$ has, for any $p > (1+\sqrt{2})\xi_0$, two positive solutions, and we define a function $\hat{q}$ by $\hat{q}(p) = q$, the largest positive one. Then we prove in Lemma 4.2 that for ξ_{max} large and $q = \hat{q}(p)$, the polynomial P has precisely three distinct positive roots, and we estimate $\bar{\xi}(p, \hat{q}(p))$. After this step, we deduce in Lemma 4.3 that for ξ_{max} sufficiently large there is at least one solution p_* to

$$R(\xi_0, p, \hat{q}(p), \xi_0) = R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0). \tag{4.16}$$

$p_* + 4i\omega\nu q_*$ is a strict local minimum for h_l^r defined in (2.10), with $l = 0$, $K_1 = i[0, \omega_{max}]$, and $n = 1$. Corollary 2.10 then states that $(p^*, q^*) = (p_*, q_*)$, which concludes the proof.

The equation $R(\xi_0, p, q, \xi_0, 0) = R(\xi_{\max}, p, q, \xi_0, 0)$ can be rewritten as an equation for the q variable,

$$-4p\xi_0(\xi_{\max} + \xi_0)\xi_{\max}^2 q^2 + 2(\xi_{\max} + \xi_0)(p^2 + \xi_0^2)\xi_{\max} q + p(p^2 - 2\xi_0\xi_{\max} - \xi_0^2) = 0. \tag{4.17}$$

The discriminant of (4.17) is

$$\Delta = \xi_{\max}^2(\xi_{\max} + \xi_0)\left[\xi_{\max}(p^4 - 6\xi_0^2 p^2 + \xi_0^4) + \xi_0\left((p^2 - \xi_0^2)^2 + 4p^4\right)\right], \tag{4.18}$$

and is positive for large $\xi_{\max}$ under the assumption $p > (1 + \sqrt{2})\xi_0$. Since the sum and the product of the roots in (4.17) is positive, there are two positive roots, and we choose $q = \hat{q}(p)$ as the larger one, *i.e.* [1]

$$\hat{q}(p) = \frac{(\xi_0^2 + p^2)\sqrt{\xi_0 + \xi_{\max}} + \sqrt{(5\xi_0 + \xi_{\max})p^4 - 2\xi_0^2(\xi_0 + 3\xi_{\max})p^2 + \xi_0^4(\xi_0 + \xi_{\max})}}{4p\xi_0\xi_{\max}\sqrt{\xi_0 + \xi_{\max}}}. \tag{4.19}$$

Lemma 4.2 *Let p be any positive real number with $p > (1 + \sqrt{2})\xi_0$, and $q = \hat{q}(p)$ defined in (4.19). Then for sufficiently large ξ_{max}, the polynomial P in (4.14) has exactly three distinct real roots. As ξ_{max} tends to infinity, the first one has a limit equal to $\sqrt{(p^2 - \xi_0^2)/2}$, the second one, $\bar{\xi}(p, \hat{q}(p))$, is equivalent to $\sqrt{p\xi_{\max}/2q_0}$, and the third one tends to infinity like $\xi_{max}/\sqrt{2}q_0$, where q_0 depends on p and ξ_0, $q_0 = \left(\xi_0^2 + p^2 + \sqrt{p^4 - 6\xi_0^2 p^2 + \xi_0^4}\right)/4p\xi_0$.*

Proof From the formula for q in (4.19), we obtain that for fixed p, we have $q \sim \frac{q_0}{\xi_{\max}}$ as $\xi_{\max} \to +\infty$. We perform the change of variables $\chi = \xi^2/\xi_0\xi_{\max}$, which transforms the equation $P(\xi) = 0$ into $\tilde{P}(\chi) = 0$ with

$$\tilde{P}(\chi) \sim 32\xi_0^3 q_0^3 \chi^3 - 16q_0\xi_0^2(\xi_{\max} - 3q_0 p)\chi^2 + 8\xi_0(p\xi_{\max} + q_0\xi_0^2 - 3q_0 p^2)\chi + 4p(\xi_0^2 - p^2).$$

$\tilde{P}$ has three real roots. Using the sum of the roots, we see that the largest one tends to infinity like $\frac{\xi_{max}}{2\xi_0 q_0^2}$, then by the second symmetric function of the roots, the middle one tends to $\frac{p}{2\xi_0 q_0}$, and finally using the product of the roots, the smallest one tends to zero like $\frac{p^2 - \xi_0^2}{2\xi_0\xi_{max}}$. From these expressions the result follows by inverting the change of variable. ∎

Lemma 4.3 *For ξ_{max} sufficiently large, there exists at least one solution $p_* > (1 + \sqrt{2})\xi_0$ to (4.16). Moreover, for any fixed p_0, if ξ_{max} is large, there is no solution in $[0, p_0]$.*

Proof For any fixed p, $R(\xi_0, p, \hat{q}(p), \xi_0, 0) < 1$ independently of ξ_{max}, and $R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0)$ tends to 1 as ξ_{max} tends to infinity. Therefore, for ξ_{max} large, $R(\xi_0, p, \hat{q}(p), \xi_0, 0) - R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0)$ is negative for any fixed p. If p tends to infinity, we have

$$R(\xi_0, p, \hat{q}(p), \xi_0, 0) = \left(\frac{p - \xi_0}{p + \xi_0}\right)^2 \sim 1 - 4\xi_0/p \quad \text{independently of } \xi_{max}. \tag{4.20}$$

On the other hand, for ξ_{max} large and fixed, if p tends to infinity, we have

$$R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0) \sim \left(\frac{p - \bar{\xi}}{p + \bar{\xi}}\right)^2 \sim 1 - 4\frac{\bar{\xi}}{p}. \tag{4.21}$$

Since $\bar{\xi} > \xi_0$, $R(\xi_0, p, \hat{q}(p), \xi_0, 0) - R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0)$ becomes positive for large p. By continuity, there exist a p_* for which this expression vanishes. ∎

We now expand p_* and $\hat{q}(p_*)$ asymptotically: by Lemma 4.3, p_* tends to infinity with ξ_{max}. Hence we can use (4.20, 4.21). Using the formula for $q = \hat{q}(p)$ in (4.19), we have that for $\xi_{\max}$, as p tends to infinity, $\hat{q}(p) \sim p/2\xi_0\xi_{max}$ and $\bar{\xi}(p, \hat{q}(p)) \sim \sqrt{\xi_0\xi_{\max}}$. Therefore, in order to match the two expansions in

[1] Formula (4.19) together with (4.16) can be useful to compute the optimal parameters, since it reduces the problem to finding a root of a scalar equation.

(4.19) leads to $q_* = \hat{q}(p_*) \sim \frac{1}{2\xi_0^{\frac{1}{4}}}\xi_{\max}^{-\frac{3}{4}}$. Finally inserting p_* and q_* into $R(\xi_0, p_*, q_*, \xi_0, 0)$ and expanding for $\xi_{\max}$ we obtain

$$R(\xi_0, p_*, q_*, \xi_0, 0) \sim 1 - 4\frac{\xi_0}{p} \sim 1 - 4\xi_0^{\frac{1}{4}}\xi_{\max}^{-\frac{1}{4}}. \tag{4.22}$$

Lemma 4.4 *$s_1 = p_* + 4\nu i\omega q_*$ is a strict local minimum for h_0^r in $\mathbf{P}_1^r$, with $K_1 = i[0, \omega_{max}]$.*

Proof For any (p, q), we define $r = \frac{1}{q}$ and $\mu(p, q, \xi_0, \xi_{max}) = \sup_{\xi \in [\xi_0, \xi_{max}]} \dfrac{1 + R(\xi, p, q, \xi_0, 0)}{1 - R(\xi, p, q, \xi_0, 0)}$, and write

$$R(\xi, p, q, \xi_0, 0) - \sup_{\xi \in [\xi_0, \xi_{max}]} R(\xi, p, q, \xi_0, 0) = 4q^2 \frac{Q(\xi, p, r, \mu)}{(\xi + p)^2 + (\xi^2 - \xi_0^2)(2\xi q + 1)^2},$$

with

$$Q(\xi, p, r, \mu) = \xi^4 - \mu r \xi^3 + (\frac{r^2}{2} - \xi_0^2)\xi^2 + \mu r(\xi_0^2 - \frac{pr}{2})\xi + r^2\frac{p^2 - \xi_0^2}{4}.$$

In the sequel, we will consider Q as a polynomial in the independent variables ξ, p, r and μ. $(p_*, r_*, \mu_* = \mu(p_*, q_*, \xi_0, \xi_{max}))$ is a solution of the system of equations

$$Q(\xi_0, p_*, r_*, \mu_*) = 0, \quad Q(\xi_{max}, p_*, r_*, \mu_*) = 0, \quad Q(\bar{\xi}, p_*, r_*, \mu_*) = \partial_\xi Q(\bar{\xi}, p_*, r_*, \mu_*) = 0.$$

Now for s_1 to be a strict local minimum for h_0^r, it is sufficient that there exists no variation $(\delta p, \delta r, \delta\mu)$ with $\delta\mu < 0$, such that $Q(\xi, p_* + \delta p, r_* + \delta r, \mu_* + \delta\mu) < 0$ for $\xi = \xi_0, \bar{\xi}, \xi_{max}$. By the Taylor formula, it suffices to prove this for $\delta p\frac{\partial Q}{\partial p}(\xi, p_*, r_*, \mu_*) + \delta r\frac{\partial Q}{\partial r}(\xi, p_*, r_*, \mu_*) + \delta\mu\frac{\partial Q}{\partial \mu}(\xi, p_*, r_*, \mu_*)$. Expanding the arguments of Q for $\xi_{\max}$ large, we have from the asymptotic results 4.22 the leading order terms. Including the next higher order terms, we obtain

$$\begin{aligned}
\bar{\xi}(p_*, q_*) &= \xi_0^{\frac{1}{2}}\xi_{max}^{\frac{1}{2}}(1 + \tfrac{1}{2}\xi_0^{\frac{1}{2}}\xi_{max}^{-\frac{1}{2}} + o(\xi_{max}^{-\frac{1}{2}})),\\
p_* &= \xi_0^{\frac{3}{4}}\xi_{max}^{\frac{1}{4}}(1 + \tfrac{1}{4}\xi_0^{\frac{1}{2}}\xi_{max}^{-\frac{1}{2}} + o(\xi_{max}^{-\frac{1}{2}})),\\
r_* &= 2\xi_0^{\frac{1}{4}}\xi_{max}^{\frac{3}{4}}(1 + \tfrac{3}{4}\xi_0^{\frac{1}{2}}\xi_{max}^{-\frac{1}{2}} + o(\xi_{max}^{-\frac{1}{2}})),\\
\mu_* &= \tfrac{1}{2}\xi_0^{-\frac{1}{4}}\xi_{max}^{\frac{1}{4}}(1 + \tfrac{5}{4}\xi_0^{\frac{1}{2}}\xi_{max}^{-\frac{1}{2}} + o(\xi_{max}^{-\frac{1}{2}})),
\end{aligned} \tag{4.23}$$

where the expansion is best obtained using the elementary symmetric functions of the roots, and then identifying terms in the expansions. The partial derivatives of Q are

$$\begin{aligned}
\frac{\partial Q}{\partial p} &= \tfrac{r^2}{2}(p - \mu\xi),\\
\frac{\partial Q}{\partial r} &= -\mu\xi^3 + r\xi^2 + \mu(\xi_0^2 - pr)\xi + \tfrac{rp^2}{2},\\
\frac{\partial Q}{\partial \mu} &= -r\xi^3 + r(\xi_0^2 - \tfrac{pr}{2})\xi.
\end{aligned} \tag{4.24}$$

Inserting the expansions (4.23) into (4.24), we obtain for the expansions of the partial derivatives

$$\begin{array}{llll}
\frac{\partial Q}{\partial p} \sim \xi_0^{\frac{5}{4}}\xi_{max}^{\frac{7}{4}}, & \frac{\partial Q}{\partial r} \sim -\frac{1}{2}\xi_0^{\frac{11}{4}}\xi_{max}^{\frac{1}{4}}, & \frac{\partial Q}{\partial \mu} \sim -2\xi_0^{\frac{9}{4}}\xi_{max}^{\frac{7}{4}}, & \text{for } \xi = \xi_0,\\
\frac{\partial Q}{\partial p} \sim -\xi_0^{\frac{3}{4}}\xi_{max}^{\frac{9}{4}}, & \frac{\partial Q}{\partial r} \sim +\frac{1}{2}\xi_0^{\frac{5}{4}}\xi_{max}^{\frac{7}{4}}, & \frac{\partial Q}{\partial \mu} \sim -4\xi_0^{\frac{7}{4}}\xi_{max}^{\frac{9}{4}}, & \text{for } \xi = \bar{\xi},\\
\frac{\partial Q}{\partial p} \sim -\xi_0^{\frac{1}{4}}\xi_{max}^{\frac{11}{4}}, & \frac{\partial Q}{\partial r} \sim -\frac{1}{2}\xi_0^{-\frac{1}{4}}\xi_{max}^{\frac{13}{4}}, & \frac{\partial Q}{\partial \mu} \sim -2\xi_0^{\frac{1}{4}}\xi_{max}^{\frac{15}{4}}, & \text{for } \xi = \xi_{max}.
\end{array} \tag{4.25}$$

Let $(\delta p, \delta r, \delta\mu)$ such that $\delta p\frac{\partial Q}{\partial p}(\xi, p_*, r_*, \mu_*) + \delta r\frac{\partial Q}{\partial r}(\xi, p_*, r_*, \mu_*) + \delta\mu\frac{\partial Q}{\partial \mu}(\xi, p_*, r_*, \mu_*) < 0$ for $\xi = \xi_0$, $\xi = \bar{\xi}$ and $\xi = \xi_{max}$. Using the expansion (4.25),we have for large ξ_{max}

$$\begin{aligned}
\xi_{max}^{\frac{3}{2}}\delta p - \tfrac{1}{2}\xi_0^{\frac{3}{2}}\delta r - 2\xi_0\xi_{max}^{\frac{3}{2}}\delta\mu &< 0,\\
-\xi_{max}^{\frac{1}{2}}\delta p + \tfrac{1}{2}\xi_0^{\frac{1}{2}}\delta r - 4\xi_0\xi_{max}^{\frac{1}{2}}\delta\mu &< 0,\\
-\xi_0^{\frac{1}{2}}\delta p - \tfrac{1}{2}\xi_{max}^{\frac{1}{2}}\delta r - 2\xi_0^{\frac{1}{2}}\xi_{max}\delta\mu &< 0.
\end{aligned} \tag{4.26}$$

For $\delta\mu < 0$, equations (4.26) imply

$$\left(\frac{\xi_{max}}{\xi_0}\right)^{\frac{3}{2}}\delta p - \frac{1}{2}\delta r < 0, \qquad -\left(\frac{\xi_{max}}{\xi_0}\right)^{\frac{1}{2}}\delta p + \frac{1}{2}\delta r < 0, \qquad -\delta p - \frac{1}{2}\left(\frac{\xi_{max}}{\xi_0}\right)^{\frac{1}{2}}\delta r < 0. \tag{4.27}$$

the second inequality we then obtain $\delta r < 0$, which together contradict the last inequality in (4.27). ■
By Corollary 2.10, we obtain $(p_*, q_*) = (p^*, q^*)$, which concludes the proof of Theorem 4.1. ■
If the algorithm is discretized in time with a time step Δt, then $\xi_{\max}$ is indeed large for $\Delta t \to 0$ and we obtain from (4.15):

Corollary 4.2 (O1 Discrete Convergence Factor Estimate without Overlap) *For Δt small, there is a unique solution of the min-max problem (4.12). The values of p^*, q^* and $R_{O1}(\xi_0, \xi_{max})$ have the following asymptotic leading order term as Δt tends to 0:*

$$p^* \sim \xi_0^{\frac{3}{4}}(2\pi\nu)^{\frac{1}{8}}\Delta t^{-\frac{1}{8}}, \qquad q^* \sim \frac{1}{2\xi_0^{\frac{1}{4}}(2\pi\nu)^{\frac{3}{8}}}\Delta t^{\frac{3}{8}}, \qquad R_{O1}(\xi_0, \xi_{max}) \sim 1 - 4\xi_0^{\frac{1}{4}}(2\pi\nu)^{-\frac{1}{8}}\Delta t^{\frac{1}{8}}.$$

Remark 4.2 *In the course of Theorem 4.1, we have proved the first assertion in Remark 2.1: for large ω_{max}, which corresponds to large K_1, the number of equioscillation points for the real problem (2.11) is actually equal to 3. For the second assertion in that remark, we show now that, when ω_{max} tends to 0, or equivalently ξ_{max} tends to ξ_0, there can not be three equioscillations points for the best approximation polynomial s_1^*: suppose there are three equioscillation points. The study of R in the first part of the proof of Theorem 4.1 shows that two of them have to be ξ_0 and ξ_{max}. Letting $\xi_{max} = \xi_0(1+\epsilon)$, with $\epsilon > 0$, we first see that p^* has to tend to ξ_0 with ξ_{max}. On the one hand, we have*

$$h(s_1^*) \leq h(\xi_0) = \frac{\xi_{max} - \xi_0}{\xi_{max} + \xi_0} \sim \frac{\epsilon}{2}.$$

and on the other hand,

$$h(s_1^*) \geq \left|\frac{f(0) - s_1^*(0)}{f(0) + s_1^*(0)}\right| = \left|\frac{p^* - \xi_0}{p^* + \xi_0}\right|,$$

which proves that p^* tends to ξ_0. Therefore it has the form $p^* = \xi_0(1 + C\epsilon) + \mathcal{O}(\epsilon^2)$ with $C \leq 1$. Inserting these values into the formula for the discriminant in (4.18) gives $\Delta \sim 8\xi_0^8(2C-1)\epsilon$, which implies $C \geq 1/2$. We now calculate from (4.19) $q^* \sim \frac{1}{2\xi_0}$. For $p = \xi_0$ and $q = \frac{1}{2\xi_0}$, the polynomial P is equal to $\frac{4}{\xi_0^3}\xi^4(\xi^2 - \xi_0^2)$, which has ξ_0 as a root. This shows that there is an extremum at ξ_0, but it is a minimum of R, since the derivative of P with respect to ξ is equal to $8\xi_0^2 > 0$.

4.2.2 The Overlapping Case

With the exponential weight, it is interesting to consider the best approximation problem for ω in $\mathbb{R}$, since this gives insight for the discrete case with limiting value ω_{max}. With the notation in Section 2, this corresponds to $l > 0$, $K_1 = i\mathbb{R}_+$, $K = i\mathbb{R}$. By Theorem 2.5, we know that a solution exists, but we loose the uniqueness and the fact that the coefficients are real. We therefore restrict our analysis to (2.12), and will use the *ad hoc* Theorem 2.11 to prove similar results as in the non-overlapping case. With the notation in (4.2), (4.1), the problem (2.12) is equivalent to finding (p_∞^*, q_∞^*) in $(\mathbb{R}_+)^2$ such that

$$\inf_{p\geq 0, q\geq 0}\sup_{\xi\geq\xi_0} R(\xi, p, q, \xi_0, L) = \sup_{\xi\geq\xi_0} R(\xi, p_\infty^*, q_\infty^*, \xi_0, L),$$

and the value of the infimum is called $R_{O1}^\infty(\xi_0, L)$. To simplify the notation, we set

$$\zeta = \frac{L\xi}{\nu}, \quad \zeta_0 = \frac{L\xi_0}{\nu}, \quad \tilde{p} = \frac{Lp}{\nu}, \quad \tilde{q} = \frac{\nu q}{L},$$

so we remove the explicit dependence on the overlap parameter L and the parameter ν of the convergence factor R given in (4.1). The value of R in the new variables ζ, $\tilde{p}$, $\tilde{q}$ and ζ_0, is

$$\tilde{R}(\zeta, \tilde{p}, \tilde{q}, \zeta_0) = R(\xi, p, q, \xi_0, L) = \frac{(\zeta - \tilde{p})^2 + (\zeta^2 - \zeta_0^2)(1 - 2\zeta\tilde{q})^2}{(\zeta + \tilde{p})^2 + (\zeta^2 - \zeta_0^2)(1 + 2\zeta\tilde{q})^2}e^{-\zeta}. \tag{4.28}$$

The new real best approximation problem is therefore to find $(\tilde{p}_\infty^*, \tilde{q}_\infty^*)$ in $(\mathbb{R}_+)^2$ such that

$$\inf_{\tilde{p}\geq 0, \tilde{q}\geq 0}\sup_{\zeta\geq\zeta_0} \tilde{R}(\zeta, \tilde{p}, \tilde{q}, \zeta_0) = \sup_{\zeta\geq\zeta_0} \tilde{R}(\zeta, \tilde{p}_\infty^*, \tilde{q}_\infty^*, \zeta_0). \tag{4.29}$$

We show now that, for small overlap L, there is a unique solution, which equioscillates at three points, and we obtain the analogon of Theorem 4.1.

lution of (4.29) is unique and equioscillates three times, i.e. $(\tilde{p}^*_\infty, \tilde{q}^*_\infty)$ *is the unique solution of*

$$\tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_0) = \tilde{R}(\zeta_2(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) = \tilde{R}(\zeta_4(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) \tag{4.30}$$

where $\zeta_2(\tilde{p}, \tilde{q})$ *denotes the second and* $\zeta_4(\tilde{p}, \tilde{q})$ *the fourth of the four distinct positive roots, ordered in increasing order, of the polynomial*

$$\begin{array}{rcl} P(\zeta) & = & 16\tilde{q}^4\zeta^8 - 32\tilde{q}^3(\tilde{q}\zeta_0^2 + 1)\zeta^6 \\ & + & (16\tilde{q} - 48\tilde{q}^2\tilde{p} + 16\tilde{q}^4\zeta_0^4 + 4 + 64\tilde{q}^3\zeta_0^2 + 8\tilde{q}^2\tilde{p}^2 + 8\tilde{q}^2\zeta_0^2 - 16\tilde{q}\tilde{p})\zeta^4 \\ & + & (-32\tilde{q}^3\zeta_0^4 + 16\tilde{q}\zeta_0^2\tilde{p} - 8\tilde{q}\zeta_0^2 + 24\tilde{q}\tilde{p}^2 - 4\zeta_0^2 - 8\tilde{p} + 16\tilde{q}^2\zeta_0^2\tilde{p} - 8\tilde{q}^2\zeta_0^4 - 8\tilde{q}^2\zeta_0^2\tilde{p}^2)\zeta^2 \\ & + & (\zeta_0^2 - \tilde{p}^2)(\zeta_0^2 + 8\tilde{q}\zeta_0^2 - \tilde{p}^2 - 4\tilde{p}). \end{array} \tag{4.31}$$

For L *small, the optimal parameters and the bound* $R^\infty_{O1}(\xi_0, L)$ *on the convergence factor, which is the common value in (4.30) at point* $(\tilde{p}, \tilde{q}) = (\tilde{p}^*_\infty, \tilde{q}^*_\infty)$*, have the expansion*

$$p^*_\infty \sim \xi_0^{\frac{4}{5}}\nu^{\frac{1}{5}}L^{-\frac{1}{5}}, \quad q^*_\infty \sim \frac{1}{2}\nu^{-\frac{3}{5}}\xi_0^{-\frac{2}{5}}L^{\frac{3}{5}}, \quad R^\infty_{O1}(\xi_0, L) \sim 1 - 4\xi_0^{\frac{1}{5}}\nu^{-\frac{1}{5}}L^{\frac{1}{5}}. \tag{4.32}$$

Proof

1. We first examine the variations of $\tilde{R}$. For fixed $\tilde{p}, \tilde{q}$, the partial derivative of $\tilde{R}$ with respect to ζ shows that the roots of P given in (4.31) determine the extrema of $\tilde{R}$. Since P is a bi-quartic in ζ with real coefficients, it has at most four positive real roots, and hence for $\zeta \geq \zeta_0 \geq 0$, $\tilde{R}$ can have at most two interior maxima. Using the change of variables $\chi = 2\tilde{q}\zeta^2$, we obtain

$$\begin{aligned} P(\zeta) = {} & \chi^4 - 4\chi^3 + (\frac{4}{\tilde{q}} - 12\tilde{p} - 4\frac{\tilde{p}}{\tilde{q}} + 2\tilde{p}^2 + \frac{1}{\tilde{q}^2})\chi^2 + (12\tilde{p}^2 - 4\frac{\tilde{p}}{\tilde{q}})\chi + \tilde{p}^2(\tilde{p}^2 + 4\tilde{p}) \\ & + y_0^2\left[-4\tilde{q}\chi^3 + (2 + 16\tilde{q})\chi^2 + (-4\tilde{q}\tilde{p}^2 + 8\tilde{q}\tilde{p} - \frac{2}{\tilde{q}} - 4 + 8\tilde{p})\chi - 2\tilde{p}(\tilde{p} + 4\tilde{q}\tilde{p} + 2)\right] \\ & + y_0^4\left[4\tilde{q}^2\chi^2 - 4\tilde{q}(1 + 4\tilde{q})\chi + 1 + 8\tilde{q}\right]. \end{aligned}$$

   The dominant part of P for $\tilde{q}$ sufficiently large, $\tilde{p}\tilde{q}$ sufficiently small, and for ζ_0 sufficiently small, is

$$P_0(\chi) = \chi^4 - 4\chi^3 + \frac{4}{\tilde{q}}\chi^2 - \frac{4\tilde{p}}{\tilde{q}}\chi + 4\tilde{p}^3.$$

   This polynomial has four real positive distinct roots χ_j, $j = 1\ldots4$, ordered in increasing order. If $1/\tilde{q}$ and $\tilde{p}\tilde{q}$ tend to 0, we have $\chi_1 \sim \tilde{q}\tilde{p}^2$, $\chi_2 \sim \tilde{p}$, $\chi_3 \sim 1/\tilde{q}$, $\chi_4 \sim 4$. By a perturbation argument, it follows that for ζ_0 sufficiently small (which corresponds to L going to zero), P has 4 real positive distinct roots as well, with the asymptotic behavior

$$\zeta_1 \sim \frac{\tilde{p}}{\sqrt{2}}, \quad \zeta_2 \sim \sqrt{\frac{\tilde{p}}{2\tilde{q}}}, \quad \zeta_3 \sim \frac{1}{\tilde{q}\sqrt{2}}, \quad \zeta_4 \sim \frac{\sqrt{2}}{\tilde{q}}.$$

2. We now show that (4.30) has a solution $(\tilde{p}_*, \tilde{q}_*)$ for ζ_0 small. We add the assumptions that $\zeta_0 = o(\tilde{p})$ as $\tilde{p}$ tends to 0, and we easily find asymptotic expansions of the three terms in (4.30),

$$\begin{array}{rclcl} R_0 & = & \tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_0) & \sim & 1 - 4\frac{\zeta_0}{\tilde{p}}, \\ R_2 & = & \tilde{R}(\zeta_2(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) & \sim & 1 - 4\sqrt{2\tilde{p}\tilde{q}}, \\ R_4 & = & \tilde{R}(\zeta_4(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) & \sim & 1 - 2\sqrt{\frac{2}{\tilde{q}}}. \end{array} \tag{4.33}$$

   The map $(\tilde{p}, \tilde{q}) \mapsto (R_2 - R_0, R_4 - R_0)$ maps a domain $(q_0 < \tilde{q} < \tilde{p}/2\zeta_0^2, 0 < \tilde{p}\tilde{q} < \epsilon_0)$ for q_0 large and ϵ_0 small, onto a neighbourhood of 0 in $\mathbb{R}^2$.

3. We now establish the asymptotic expansions for $(\tilde{p}_*, \tilde{q}_*)$. They are easily found by equating the expansions in (4.33). We solve

$$\frac{\zeta_0}{\tilde{p}} = \sqrt{2\tilde{p}\tilde{q}} = \frac{1}{\sqrt{2\tilde{q}}},$$

$$\tilde{p}_* \sim \zeta_0^{4/5}, \quad \tilde{q}_* \sim \frac{1}{2}\zeta_0^{-2/5}, \tag{4.34}$$

and (4.32) by the change of variables. In particular the assumption $\zeta_0 = o(\tilde{p})$ in item 2 is validated.

4. We now prove that for L sufficiently small, $(\tilde{p}_*, \tilde{q}_*)$ is a strict local minimum for the best approximation problem (4.29). The pair $(\tilde{p}_*, \tilde{q}_*)$ is a strict local minimum if there exists no variation $(\delta p, \delta q)$ such that $\tilde{R}(\zeta, \tilde{p}_* + \delta p, \tilde{q}_* + \delta q, \zeta_0) < \tilde{R}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0)$ for $\zeta = \zeta_0, \zeta_2, \zeta_4$. By the Taylor formula, it suffices to prove that there is no variation $(\delta p, \delta q)$, such that $\delta p \frac{\partial \tilde{R}}{\partial p}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) + \delta q \frac{\partial \tilde{R}}{\partial q}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) < 0$ for $\zeta = \zeta_0, \zeta_2, \zeta_4$. For ζ_0 small, expanding the arguments of $\tilde{R}$, we have from (1) and (4.34) the leading order terms in the expansion. Including the next higher order terms, we find

$$\begin{array}{rclrcl} \tilde{p}_* & \sim & \zeta_0^{\frac{4}{5}}(1 - \frac{1}{15}\zeta_0^{\frac{2}{5}}), & \tilde{q}_* & \sim & \frac{1}{2}\zeta_0^{-\frac{2}{5}}(1 - \frac{7}{10}\zeta_0^{\frac{2}{5}}), \\ \zeta_2 & \sim & \zeta_0^{\frac{3}{5}}(1 + \frac{2}{15}\zeta_0^{\frac{2}{5}}), & \zeta_4 & \sim & 2\zeta_0^{\frac{1}{5}}(1 + \frac{1}{10}\zeta_0^{\frac{2}{5}}). \end{array}$$

Inserting these expansions into the expressions of the derivatives of $\tilde{R}$, we get

$$\begin{array}{rclrcl} \frac{\partial \tilde{R}}{\partial p}(\zeta_0, \tilde{p}_*, \tilde{q}_*, \zeta_0) & \sim & 4\zeta_0^{\frac{3}{5}}, & \frac{\partial \tilde{R}}{\partial q}(\zeta_0, \tilde{p}_*, \tilde{q}_*, \zeta_0) & = & 0, \\ \frac{\partial \tilde{R}}{\partial p}(\zeta_2, \tilde{p}_*, \tilde{q}_*, \zeta_0) & \sim & -2\zeta_0^{\frac{3}{5}}, & \frac{\partial \tilde{R}}{\partial q}(\zeta_2, \tilde{p}_*, \tilde{q}_*, \zeta_0) & \sim & -4\zeta_0^{\frac{3}{5}}, \\ \frac{\partial \tilde{R}}{\partial p}(\zeta_4, \tilde{p}_*, \tilde{q}_*, \zeta_0) & \sim & -\frac{1}{2}\zeta_0^{\frac{1}{5}}, & \frac{\partial \tilde{R}}{\partial q}(\zeta_4, \tilde{p}_*, \tilde{q}_*, \zeta_0) & \sim & 4\zeta_0^{\frac{3}{5}}. \end{array} \tag{4.35}$$

Let $\mathcal{E}$ be the set of vectors $(\delta p, \delta q)$ such that $\delta p \frac{\partial \tilde{R}}{\partial p}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) + \delta q \frac{\partial \tilde{R}}{\partial q}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) < 0$ for $\zeta = \zeta_0, \zeta_2, \zeta_4$. We need to prove that $\mathcal{E}$ is empty. For small ζ_0, $\mathcal{E}$ can be obtained using the expansion (4.35):

$$4\zeta_0^{\frac{3}{5}}\delta p < 0, \quad -2\zeta_0^{\frac{3}{5}}\delta p - 4\zeta_0^{\frac{3}{5}}\delta q < 0, \quad -\frac{1}{2}\zeta_0^{\frac{1}{5}}\delta p + 4\zeta_0^{\frac{3}{5}}\delta q < 0. \tag{4.36}$$

The first inequality in (4.36) implies $\delta p < 0$, while adding the second and the third inequality in (4.36) yields $\delta p > 0$, which is a contradiction, and thus the set $\mathcal{E}$ is empty.

Using the uniqueness in Theorem 2.11, we obtain $(\tilde{p}_\infty^*, \tilde{q}_\infty^*) = (\tilde{p}_*, \tilde{q}_*)$, which concludes the proof. ∎

In Figure 2, we show the convergence factors $R_{T1}^\infty(\xi_0, L)$ and $R_{O1}^\infty(\xi_0, L)$ for an example with $\xi_0 = 1$, $L = 0.08$ and $\nu = 0.2$ from the numerical section.

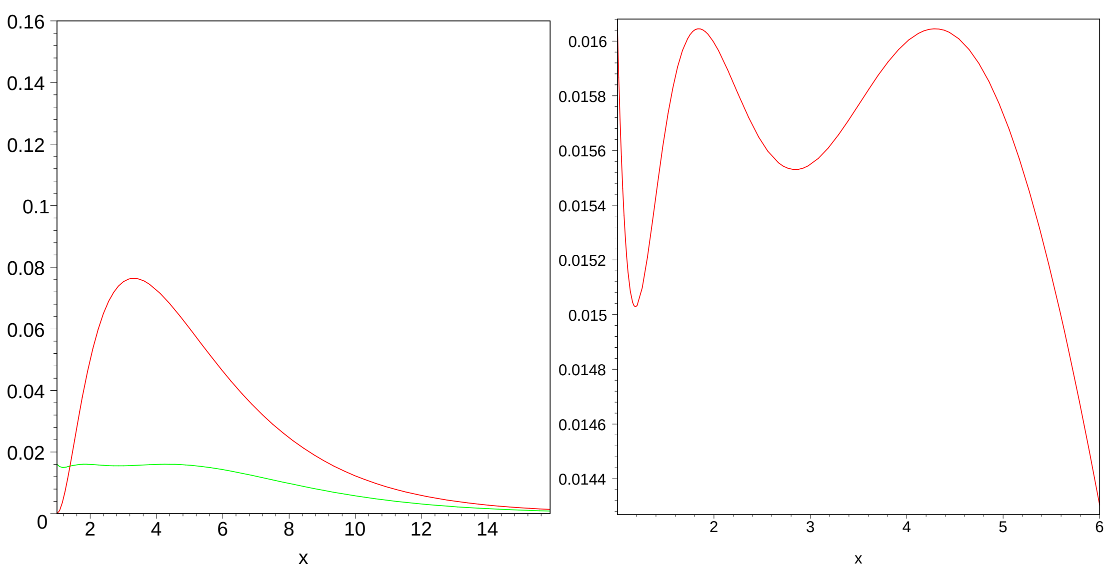

Figure 2: Convergence factors R_{T1}^∞ and R_{O1}^∞ for an overlapping example from the numerical section on the left, and zoom on the right showing the equioscillation at the optimal solution.

One can see on the left the much better performance of the optimized first order transmission conditions compared to the first order Taylor transmission conditions, and also the equioscillation of the optimal exponential take over.

Theorem 4.3 gives the parameters p^* and q^* to choose in the first order transmission conditions of the optimized Schwarz waveform relaxation algorithm at the continuous level to get the best convergence factor, which is $1 - O(L^{\frac{1}{5}})$, and therefore is significantly better than the best result achievable with optimized Robin conditions [11], which led to a convergence factor $1 - O(L^{\frac{1}{3}})$.

In Figure 3, we show the first few iterations, at the end of the time interval, of the classical and optimized Schwarz waveform relaxation algorithm with first order optimized transmission conditions according to Theorem 4.3 for a model problem.

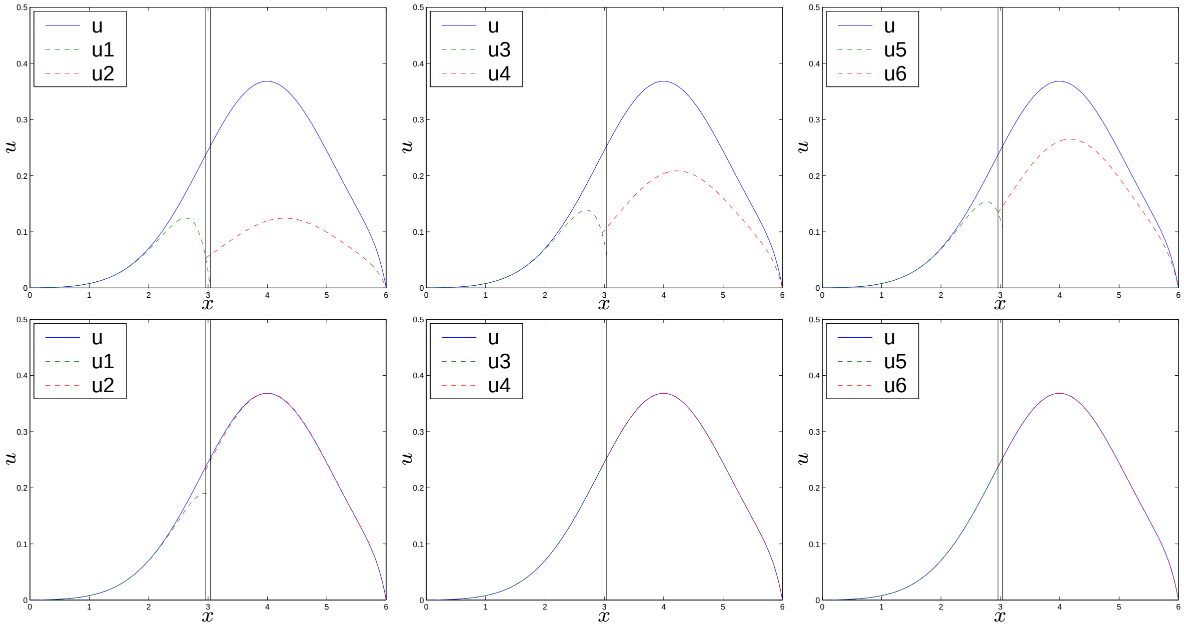

Figure 3: From left to right, the iterates $u_1^k(x,T)$ and $u_2^{k+1}(x,T)$ (dashed) at the end of the time interval $t = T$ for $k = 1, 3, 5$ for an example from the numerical section, together with the exact solution (solid). Top row the classical Schwarz waveform relaxation algorithm, and bottom row the optimized one.

This experiment shows well that the new transmission conditions improve the convergence behavior tremendously, they are very effective to transport the convected solution from left to right across the artificial interfaces between subdomains.

As we have seen earlier, in a numerical setting, not all the frequencies are present. We thus have to address the question again if the maximum of the convergence factor attained at y_4 is relevant in a computation. Letting $L = C_1\Delta x$ and $\Delta t = C_2 \Delta x^\beta$, the maximum numerical frequency we can expect on the time discretization grid leads from (4.5) to a bound on ζ, $\zeta_0 \leq \zeta \leq \zeta_{\max}$, where $\zeta_{\max}$ has the expansion

$$\zeta_{\max} = \frac{Lx_{\max}}{\nu} = C_1\Delta x \sqrt{\frac{\sqrt{x_0^4 + \left(\frac{4\nu\pi}{C_2\Delta x^\beta}\right)^2} + x_0^2}{2}} = C_1\sqrt{\frac{2\pi}{\nu C_2}}\Delta x^{1-\frac{\beta}{2}} + O(\Delta x^{1+\frac{\beta}{2}}).$$

Now ζ_4 from the optimization in (4.30) satisfies for L (and thus ζ_0) small

$$\zeta_4 \sim 2\zeta_0^{\frac{1}{5}} = 2\left(\frac{\xi_0 C_1}{\nu}\right)^{\frac{1}{5}} \Delta x^{\frac{1}{5}}.$$

Hence, if $1 - \frac{\beta}{2} = \frac{1}{5}$ *i.e.* $\beta = \frac{8}{5}$ and if C_1 is equal to the critical value $C_c = \nu^{\frac{3}{8}}\xi_0^{\frac{1}{4}}\left(\frac{2C_2}{\pi}\right)^{\frac{5}{8}}$, the numerical $\zeta_{\max}$ and ζ_4 from the optimization are asymptotically at the same location, which represents the boundary between the usefulness of the continuous optimization result (4.30) on an unbounded domain, and the optimization on the compact set $[0, \omega_{max}]$, for which the analysis in Section 2.2 becomes relevant, as we sufficiently small overlap L. By Theorem 2.8, s_1^* has real coefficients. Therefore, (p^*, q^*) is the unique pair of real numbers such that

$$\inf_{p,q\in\mathbb{R}} \sup_{\xi_0\le\xi\le\xi_{max}} R(\xi,p,q,\xi_0,L) = \sup_{\xi_0\le\xi\le\xi_{max}} R(\xi,p^*,q^*,\xi_0,L), \tag{4.37}$$

where we denote the infimum by $R_{O1}(\xi_0,\xi_{max},L)$, which is also equal to $\left(\delta_1(\frac{L}{2\nu})\right)^2$.

Lemma 4.5 *The solution (p^*, q^*) of the min-max problem (4.37) satisfies $p^* > 0$ and $q^* \geq 0$.*

Proof By Theorems 2.1, 2.3 and 2.8, there is a unique real number p_0^* in $\mathbf{P}_0$ such that

$$\inf_{p\in\mathbb{R}} \sup_{\xi_0\le\xi\le\xi_{max}} R(\xi,p,0,\xi_0,0) = \sup_{\xi_0\le\xi\le\xi_{max}} R(\xi,p_0^*,0,\xi_0,0),$$

and the value of the infimum is δ_0^2. Furthermore, since $\delta_0 < 1$, p_0^* is positive. If (p^*, q^*) is a solution of the min-max problem (4.29), we have

$$\begin{aligned} R(\xi_0,p^*,q^*,\xi_0,L) = \frac{(\xi_0-p^*)^2}{(\xi_0+p^*)^2}e^{-\frac{L}{\nu}\xi_0} &\le \max_{\xi_0\le\xi\le\xi_{max}} R(\xi,p^*,q^*,\xi_0,L) \\ &\le \max_{\xi_0\le\xi\le\xi_{max}} R(\xi,p_0^*,0,\xi_0,L) \le \max_{\xi_0\le\xi\le\xi_{max}} R(\xi,p_0^*,0,\xi_0,0)e^{-\frac{L}{\nu}\xi_0} \\ &\le \delta_0^2 e^{-\frac{L}{\nu}\xi_0} < e^{-\frac{L}{\nu}\xi_0}, \end{aligned}$$

with the notation from (2.1), which can only hold if $p^* > 0$. To prove that $q^* \geq 0$, we note that for negative q, we have for any $\xi \geq \xi_0$ from (4.1) $R(\xi,p,q,\xi_0,L) \geq R(\xi,p,-q,\xi_0,L)$, which can be seen by expanding the numerator of $R(\xi,p,q,\xi_0,L) - R(\xi,p,-q,\xi_0,L)$. ∎

Theorem 4.4 (O1 Discrete Convergence Factor Estimate with Overlap) *If $L = C_1\Delta x$ and $\Delta t = C_2\Delta x^\beta$, for Δx sufficiently small, we have the following asymptotic behaviors:*

1. *For $\beta > \frac{8}{5}$, or $\beta = \frac{8}{5}$ and $C_1 > C_c$,*

$$R_{O1}(\xi_0,\xi_{max},L) \sim 1 - 4\left(\tfrac{C_1\xi_0}{\nu}\right)^{\frac{1}{5}}\Delta x^{\frac{1}{5}}, \quad p^* \sim \left(\tfrac{\xi_0^4\nu}{C_1}\right)^{\frac{1}{5}}\Delta x^{-\frac{1}{5}}, \quad q^* \sim 2C_1^{\frac{3}{5}}\left(\tfrac{\nu}{\xi_0}\right)^{\frac{2}{5}}\Delta x^{\frac{3}{5}},$$

where $C_c = \nu^{\frac{3}{8}}\xi_0^{\frac{1}{4}}\left(\frac{2C_2}{\pi}\right)^{\frac{5}{8}}$.

2. *For $\beta = \frac{8}{5}$ and $C_1 \leq C_c$,*

$$R_{O1}(\xi_0,\xi_{max},L) \sim 1 - \left(\tfrac{4C_1\xi_0}{\tilde{C}_p\nu}\right)\Delta x^{\frac{1}{5}}, \quad p^* \sim \tfrac{\tilde{C}_p\nu}{C_1}\Delta x^{-\frac{1}{5}}, \quad q^* \sim 2\tfrac{\xi_0^2C_1^3}{\tilde{C}_p^3\nu^2}\Delta x^{\frac{3}{5}},$$

where $\tilde{C}_p$ is the unique positive root of the polynomial

$$\tilde{P}(\xi) = 2\nu^3C_2\xi^4 + C_1\pi\xi_0^2\xi - 2\xi_0^3C_1^4\sqrt{\frac{2\pi C_2}{\nu}}.$$

3. *Finally for $0 < \beta < \frac{8}{5}$, we have*

$$R_{O1}(\xi_0,\xi_{max},L) \sim 1 - 2\left(\tfrac{2^7C_2\xi_0^2}{\pi\nu}\right)^{\frac{1}{8}}\Delta x^{\frac{\beta}{8}}, \quad p^* \sim \left(\tfrac{2\pi\nu\xi_0^6}{C_2}\right)^{\frac{1}{8}}\Delta x^{-\frac{\beta}{8}}, \quad q^* \sim \left(\tfrac{(2\nu)^5C_2^3}{\xi_0^2\pi^3}\right)^{\frac{1}{8}}\Delta x^{\frac{3\beta}{8}}.$$

Proof We use here the notation introduced for Theorem 4.3, see (4.28), and consider the minmax problem in the form

$$\inf_{\tilde{p}\in\mathbb{R},\tilde{q}\in\mathbb{R}} \sup_{\zeta_0\le\zeta\le\zeta_{max}} \tilde{R}(\zeta,\tilde{p},\tilde{q},\zeta_0) = \sup_{\zeta_0\le\zeta\le\zeta_{max}} \tilde{R}(\zeta,\tilde{p}^*,\tilde{q}^*,\zeta_0). \tag{4.38}$$

parameters $(\tilde p^*_\infty, \tilde q^*_\infty)$, since in the first case, $\zeta_{max} > \zeta_4(\tilde p^*_\infty, \tilde q^*_\infty)$.

For the two other cases, we have asymptotically $\zeta_3(\tilde p^*_\infty, \tilde q^*_\infty) \le \zeta_{max} \le \zeta_4(\tilde p^*_\infty, \tilde q^*_\infty)$, and the proof follows the same steps as before: we first show the existence of $(\tilde p_*, \tilde q_*)$, such that $\tilde R(\zeta, \tilde p, \tilde q, \zeta_0)$ equioscillates at the three points ζ_0, $\zeta_2(\tilde p, \tilde q)$ and ζ_{max}. We then determine the expansions of $(\tilde p_*, \tilde q_*), \zeta_2(\tilde p_*, \tilde q_*)$, deduce that $(\tilde p_*, \tilde q_*)$ is a strict local minimum for h_l in $\mathbf{P}^r_n$, and finally conclude that $(\tilde p_*, \tilde q_*) = (\tilde p^*, \tilde q^*)$.

We work with ζ_0 as the small parameter: let $C_m = C_1\left(\frac{2\pi}{\nu C_2}\right)^{1/2}\left(\frac{\nu}{C_1 \xi_0}\right)^{1-\beta/2}$, so that $\zeta_{max} \sim C_m \zeta_0^{1-\beta/2}$. To prove the second and third result of the theorem, we need to study solutions of

$$\tilde R(\zeta_0, \tilde p, \tilde q, \zeta_0) = \tilde R(\zeta_2(\tilde p, \tilde q), \tilde p, \tilde q, \zeta_0) = \tilde R(\zeta_0, \tilde p, \tilde q, \zeta_{max}) \tag{4.39}$$

for ζ_0 small. Let $R_0 := \tilde R(\zeta_0, \tilde p, \tilde q, \zeta_0)$, $R_2 := \tilde R(\zeta_2(\tilde p, \tilde q), \tilde p, \tilde q, \zeta_0)$ and $R_{max} := \tilde R(\zeta_0, \tilde p, \tilde q, \zeta_{max})$. A direct computation gives for $\tilde q$ large, and $\tilde p \tilde q$ and ζ_0 small,

$$R_{max} \sim 1 - 4\left[\frac{1}{2q\zeta_{max}} + \frac{\zeta_{max}}{4}\right] \sim 1 - 4\left[\frac{1}{2q}\frac{\zeta_0^{\beta/2-1}}{C_m} + \frac{C_m\,\zeta_0^{1-\beta/2}}{4}\right].$$

Using the expansions from (4.33),

$$R_0 \sim 1 - 4\frac{\zeta_0}{\tilde p}, \quad R_2 \sim 1 - 4\sqrt{2\tilde p \tilde q},$$

we see first, by the Implicit Function Theorem, as in the proof of Theorem 4.3, that there exists a solution $(\tilde p_*, \tilde q_*)$ to (4.39). We find their behavior at infinity by equaling R_0, R_2 and R_{max}, which gives the system of equations

$$C_m \zeta_0^{4-\beta/2} \sim \frac{C_m^2}{4}\tilde p \zeta_0^{4-\beta} + \tilde p^4, \quad \tilde q \sim \frac{\zeta_0^2}{2\tilde p^3}.$$

For $\beta = 8/5$, the two terms on the right in the first equation are balanced, which leads to $\tilde p_* \sim C\zeta_0^{4/5}$, where C is the unique positive root [2] of $C_m = (C^3 + C_m^2/4)C$ and $\tilde q_* \sim \frac{1}{2C^2}\zeta_0^{-2/5}$. For $\beta < 8/5$, the dominant term is $\tilde p^4$, from which we find $\tilde p_* \sim C_m^{1/4}\zeta_0^{1-\beta/2}$. Using the second equation, we obtain $\tilde q_* \sim \frac{1}{2}C_m^{-3/4}\zeta_0^{-1+\frac{3\beta}{8}}$. We now expand the partial derivatives of $\tilde R$ to show that, for L sufficiently small, $(\tilde p_*, \tilde q_*)$ is a strict local minimum for the best approximation problem (4.38). For R_0, we obtain, since ζ_0 is negligible with respect to p,

$$\frac{\partial \tilde R}{\partial \tilde p}(\zeta_0, \tilde p_*, \tilde q_*, \zeta_0) \sim 4C_m^{-1/2}\zeta_0^{-1+\beta/4}, \quad \frac{\partial \tilde R}{\partial \tilde q}(\zeta_0, \tilde p_*, \tilde q_*, \zeta_0) = 0.$$

For R_2, we use that $\zeta_0 \ll \tilde p_* \ll \zeta_2 \ll \zeta_{max}$, and $\zeta_2 \tilde q_* \sim \frac{1}{2}C_m^{-1/4}\zeta_0^{\beta/8}$, to obtain

$$\frac{\partial \tilde R}{\partial \tilde p}(\zeta_2, \tilde p_*, \tilde q_*, \zeta_0) \sim -2C_m^{-1/2}\zeta_0^{-1+\beta/4}, \quad \frac{\partial \tilde R}{\partial \tilde q}(\zeta_2, \tilde p_*, \tilde q_*, \zeta_0) \sim -2C_m^{1/2}\zeta_0^{1-\beta/4}.$$

For R_{max}, we use $\zeta_{max}\tilde q_* \sim \frac{C'}{2}\zeta_0^{-\beta/8}$ with $C' = C_m^{1/4}$ for $\beta < 8/5$ and $C' = C_m/C^2$ for $\beta = 8/5$,

$$\frac{\partial \tilde R}{\partial p}(\zeta_{max}, \tilde p_*, \tilde q_*, \zeta_0) \sim -\zeta_{max}^{-3}\tilde q_*^{-2} \sim -4C_m^{-1}C'^{-2}\zeta_0^{-1+3\beta/4},$$

$$\frac{\partial \tilde R}{\partial q}(\zeta_{max}, \tilde p_*, \tilde q_*, \zeta_0) \sim 2\zeta_{max}^{-1}\tilde q_*^{-2} \sim 8C_m C'^{-2}\zeta_0^{1-\beta/4}.$$

After proceeding as in point 4 of the proof of Theorem 4.3, we use Corollary 2.10 to conclude that $(\tilde p^*, \tilde q^*) = (\tilde p_*, \tilde q_*)$, and we have the asymptotic expansion

$$R_{O1}(\xi_0, \xi_{max}, L) \sim 1 - 4\frac{\zeta_0^{\beta/2}}{C_m^{1/4}}.$$

[2]This is a polynomial equation of fourth degree which is actually the first fourth degree equation which has been solved by Lodovico Ferrari in 1545. Note that all equations in the text resume to polynomials of degree at most 4, and as such can be solved by radicals, using Del Ferro/Tartaglia/Cardan formulas [3].

$$\zeta_0 \sim \zeta_0, \quad \zeta_1 \sim \frac{C_m^{1/4}}{\sqrt{2}} \zeta_0^{1-\beta/8}, \quad \zeta_2 \sim C_m^{1/2} \zeta_0^{1-\beta/4}, \quad \zeta_3 \sim \sqrt{2} C_m^{3/4} \zeta_0^{1-3\beta/8}, \quad \zeta_{max} \sim C_m \zeta_0^{1-\beta/2},$$

■

4.3 Summary and Extension to Higher Dimensions

To summarize the results of this section, and to permit an easy lookup of the parameters p and q to be used in practice, we show in Table 1 an overview of the performance one can obtain with the various choices of the parameter p and q in the transmission conditions (3.11) of the new Schwarz waveform relaxation algorithm in one dimension.

method	convergence factor	parameter p	parameter q
Taylor no overlap	$1 - O(\sqrt{\Delta t})$	$\sqrt{a^2 + 4\nu b}$	$\frac{2\nu}{\sqrt{a^2+4\nu b}}$
Optimized no overlap	$1 - O(\Delta t^{\frac{1}{8}})$	$(2\nu\pi(a^2 + 4\nu b)^3)^{\frac{1}{8}} \Delta t^{-\frac{1}{8}}$	$(\pi^3(a^2 + 4\nu b))^{-\frac{1}{8}} (2\nu)^{\frac{5}{8}} \Delta t^{\frac{3}{8}}$
Taylor overlap Δx, $\beta \geq 1$	$1 - O(\sqrt{\Delta x})$	$\sqrt{a^2 + 4\nu b}$	$\frac{2\nu}{\sqrt{a^2+4\nu b}}$
Taylor overlap Δx, $\beta < 1$	$1 - O(\Delta x^{\frac{\beta}{2}})$		
Optimized overlap Δx, $\beta > \frac{8}{5}$	$1 - O(\Delta x^{\frac{1}{5}})$	$(\nu(a^2 + 4\nu b)^2)^{\frac{1}{5}} \Delta x^{-\frac{1}{5}}$	$2\nu^{\frac{2}{5}} (a^2 + 4\nu b)^{-\frac{1}{5}} \Delta x^{\frac{3}{5}}$
Optimized overlap Δx, $\beta < \frac{8}{5}$	$1 - O(\Delta x^{\frac{\beta}{8}})$	$(2\nu\pi(a^2 + 4\nu b)^3)^{\frac{1}{8}} \Delta x^{-\frac{\beta}{8}}$	$(2\nu)^{\frac{5}{8}} (\pi^3(a^2 + 4\nu b))^{-\frac{1}{8}} \Delta x^{\frac{3\beta}{8}}$

Table 1: Summary of the asymptotic convergence factors for the parameter choices in the first order transmission conditions in one dimension, for $\Delta t = \Delta x^\beta$.

In higher dimension, without showing the details of the derivation, the Taylor transmission conditions lead to the parameters $p_T = \sqrt{a^2 + 4\nu b}$ and $q_T = \frac{2\nu}{\sqrt{a^2+4\nu b}}$ with associated convergence factor $1 - O(\Delta x)$ in the case without overlap, and $1 - O(\sqrt{\Delta x})$ in the case with overlap $O(\Delta x)$. Even if we do not have the complete analysis in this general case for the optimized problem (*i.e.* the equivalent of Theorems 4.1, 4.3 and 4.2), we can still give formally the order of magnitude of the various quantities. The optimal parameters in the transmission conditions are for the non-overlapping case asymptotically given by $p = C_p \Delta x^{-\frac{1}{4}}$ and $q = C_q \Delta x^{\frac{3}{4}}$, which leads to an optimized convergence factor $1 - O(\Delta x^{\frac{1}{4}})$ of the associated optimized Schwarz waveform relaxation algorithm. The constants C_p and C_q depend on the problem parameters and the spatial dimension $n \geq 2$ of the problem (3.1), as shown in Table 2.

1	$\begin{cases}\bar\nu_1 \le \frac12 \text{ and } \nu > \frac12\\ \bar\nu_1 > \frac12 \text{ and } \nu > \bar\nu_2\end{cases}$	$\left(\frac{\nu\pi(a^2+4\nu b)^{\frac32}\sqrt{n-1}}{2}\right)^{\frac14}$	$\left(\frac{8\nu}{\pi^3(n-1)^{\frac32}\sqrt{a^2+4\nu b}}\right)^{\frac14}$
	$\bar\nu_1 < \nu \le \frac12$	$\left(\frac{\pi\sqrt{(a^2+4\nu b)^3(n-1)}}{4}\right)^{\frac14}$	$\left(\frac{4}{\pi^3\sqrt{(a^2+4\nu b)(n-1)^3}}\right)^{\frac14}$
	$\begin{cases}\bar\nu_1 \le \frac12 \text{ and } \nu \le \bar\nu_1\\ \bar\nu_1 > \frac12 \text{ and } \nu \le \bar\nu_2\end{cases}$	$\left(\frac{8\nu\pi(a^2+4\nu b)^2(n-1)}{(8\nu+\sqrt{(a^2+4\nu b)(n-1)})^2}\right)^{\frac14}$	$\left(\frac{128\nu}{\pi^3(n-1)(8\nu+\sqrt{(a^2+4\nu b)(n-1)})^2}\right)^{\frac14}$
2	$\begin{cases}\nu > \frac12 \text{ and } n \le 5\\ \nu > \bar\nu_6 \text{ and } n \ge 6\end{cases}$	$\left(\frac{\nu^3(a^2+4\nu b)^3(\zeta^4+16\pi^2)^2}{2(\sqrt{\nu^2\zeta^4+\pi^2}+\nu\zeta^2)(\zeta^2+4\sqrt{\nu^2\zeta^4+\pi^2}-4\nu\zeta^2)^2}\right)^{\frac18}$	$\left(\frac{8(\sqrt{\nu^2\zeta^4+\pi^2}+\nu\zeta^2)^3(\zeta^2+4\sqrt{\nu^2\zeta^4+\pi^2}-4\nu\zeta^2)^6}{\nu(a^2+4\nu b)(\zeta^4+16\pi^2)^6}\right)^{\frac18}$
	$\frac12 < \nu \le \bar\nu_6$ and $n \ge 6$	$\left(\frac{\pi\nu^3(a^2+4\nu b)^3(\pi^2(n-1)^2+16)^2}{2(\pi(n-1)(1-4\nu)+4w)^2(\nu\pi(n-1)+w)}\right)^{\frac18}$	$\left(\frac{8(\pi(n-1)(1-4\nu)+4w)^6(\nu\pi(n-1)+w)^3}{\pi^3\nu(a^2+4\nu b)(\pi^2(n-1)^2+16)^6}\right)^{\frac18}$
	$\bar\nu_5 < \nu \le \frac12$ and $2 \le n \le 5$	$(2\nu\pi(a^2+4\nu b)^3)^{\frac18}$	$\left(\frac{1}{2048(\nu\pi)^3(a^2+4\nu b)}\right)^{\frac18}$
	$\begin{cases}\bar\nu_4 < \nu \le \bar\nu_5 \text{ and } 2 \le n \le 5\\ \bar\nu_4 < \nu \le \frac12 \text{ and } n \ge 6\end{cases}$	$\left(\frac{\pi\nu(a^2+4\nu b)^3(\pi^2(n-1)^2+16)^2}{8(\pi(n-1)(1-4\nu)+4w)^2(\nu\pi(n-1)+w)}\right)^{\frac18}$	$\left(\frac{2(\pi(n-1)(1-4\nu)+4w)^6(\nu\pi(n-1)+w)^3}{\pi^3\nu^3(a^2+4\nu b)(\pi^2(n-1)^2+16)^6}\right)^{\frac18}$
	$\nu \le \bar\nu_4$ and $n \ge 2$	$\left(\frac{\pi\sqrt{(n-1)(a^2+4\nu b)^3}}{4}\right)^{\frac14}$	$\left(\frac{4}{\pi^3\sqrt{(n-1)^3(a^2+4\nu b)}}\right)^{\frac14}$

Table 2: Summary of the constants in the asymptotically optimized parameters $p = C_p\Delta x^{-\frac14}$ and $q = C_q\Delta x^{\frac34}$ in dimension $n \ge 2$ in the non-overlapping case, for $\Delta t = \Delta x^\beta$, $\beta = 1, 2$. The constants $\bar\nu_1$ up to $\bar\nu_6$, ζ and w are defined in the text.

In the table, ζ represents the smallest positive root of the polynomial

$$P(\zeta) = 3\pi^2\nu^2(8\nu-1)\zeta^3 - 4\pi^4(1-4\nu-100\nu^2+320\nu^3)\zeta^2 + 128\pi^6(48\nu^3+3-12\nu-10\nu^2)\zeta - 1024\pi^8(2\nu-1)^2,$$

$w = \sqrt{\pi^2\nu^2(n-1)^2+1}$, and the other constants are given by given by $\bar\nu_1 = \sqrt{n-1}\frac{b\sqrt{n-1}+\sqrt{b^2(n-1)+16a^2}}{32}$, $\bar\nu_2$ is the root of the equation $\nu = \frac12((a^2+4\nu b)(n-1))^{\frac14} - \frac18((a^2+4\nu b)(n-1))^{\frac12}$, $\bar\nu_2 \sim \frac{a^2\sqrt{a\sqrt{n-1}}(4-\sqrt{a\sqrt{n-1}})}{2(4a^2-2b\sqrt{a\sqrt{n-1}}+ab\sqrt{n-1})}$, $\bar\nu_3 = \frac{1}{32}\pi(n-1)$,

$$\begin{aligned}
\bar\nu_4 &= \frac{\pi(n-1)\left(\pi^5(n-1)^5+80\pi^3(n-1)^3+512\pi(n-1)+\sqrt{(3\pi^2(n-1)^2+16)(\pi^2(n-1)^2+16)^4}\right)}{16(\pi^6(n-1)^6+56\pi^4(n-1)^4+640\pi^2(n-1)^2+2048)},\\
\bar\nu_5 &= \frac{4096-2048\pi(n-1)+256\pi^2(n-1)^2+128\pi^3(n-1)^3-16\pi^4(n-1)^4-\pi^6(n-1)^6+\sqrt{d}}{1024\pi^3(n-1)^3},\\
d &= (\pi(n-1)-4)(\pi^3(n-1)^3+4\pi^2(n-1)^2+48\pi(n-1)-64)(\pi^2(n-1)^2+16)^4,
\end{aligned}$$

and $\bar\nu_6 = \bar\nu_6(n)$ is defined by equalizing the constant C_p (or C_q) of the first two cases of $\beta = 2$ in Table 2, and is shown graphically, together with the other constants, in Figure 4.

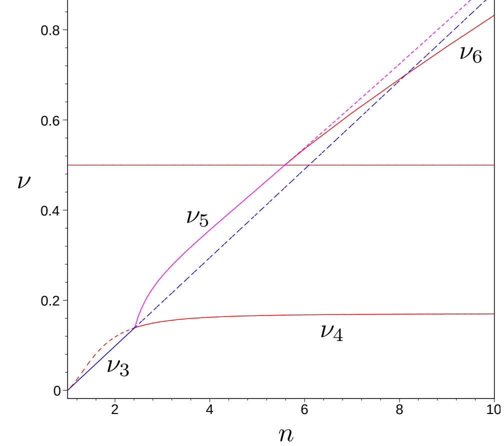

Figure 4: Regions in the n-ν plane where the different constants C_p and C_q of the optimized parameters in dimension $n \geq 2$ apply according to Table 2.

In the case with overlap, the optimal parameters in the transmission conditions are asymptotically given by $p = C_p \Delta x^{-\frac{1}{5}}$ and $q = C_q \Delta x^{\frac{3}{5}}$, where the constants C_p and C_q depend on the problem parameters, as shown in Table 3.

β	ν	C_p	C_q
1	$\nu > \frac{1}{2}$	$(\frac{1}{4}\nu(a^2+4\nu b)^2)^{\frac{1}{5}}$	$\left(\frac{64\nu^2}{(a^2+4\nu b)}\right)^{\frac{1}{5}}$
1	$\nu \leq \frac{1}{2}$	$\left(\frac{(a^2+4\nu b)^2}{8}\right)^{\frac{1}{5}}$	$\left(\frac{16}{a^2+4\nu b}\right)^{\frac{1}{5}}$
2	$\nu > \frac{1}{2}$	$(2\nu^2(a^2+4\nu b)^2)^{\frac{1}{5}}$	$\left(\frac{1}{8\nu(a^2+4\nu b)}\right)^{\frac{1}{5}}$
2	$\frac{1}{8} < \nu \leq \frac{1}{2}$	$(\nu(a^2+4\nu b)^2)^{\frac{1}{5}}$	$\left(\frac{1}{32\nu^3(a^2+4\nu b)}\right)^{\frac{1}{5}}$
2	$\nu \leq \frac{1}{8}$	$\left(\frac{(a^2+4\nu b)^2}{8}\right)^{\frac{1}{5}}$	$\left(\frac{16}{a^2+4\nu b}\right)^{\frac{1}{5}}$

Table 3: Summary of the constants in the optimized asymptotic parameters $p = C_p \Delta x^{-\frac{1}{5}}$ and $q = C_q \Delta x^{\frac{3}{5}}$ for the case with overlap $L = \Delta x$ in dimension $n \geq 2$ for $\Delta t = \Delta x^{\beta}$.

The optimized convergence factor of the associated algorithm with this choice is given by $1 - O(\Delta x^{\frac{1}{5}})$. It is interesting to note that in the case with overlap, the results are independent of the dimension for $n \geq 2$.

5 Well-posedness and convergence of the Schwarz waveform relaxation algorithms

For the analysis in this Section, we rely on the theory of weak solution in Sobolev spaces by a Galerkin method, see [2] and [20]. A weak solution of (3.1) is defined to be a $u \in \mathcal{C}(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))$, such that, for any v in $H^1(\Omega)$, we have

$$\frac{d}{dt}(u,v) + \frac{1}{2}\big(((\boldsymbol{a}\cdot\boldsymbol{\nabla})u,v) - ((\boldsymbol{a}\cdot\boldsymbol{\nabla})v,u)\big) + \nu(\nabla u,\nabla v) + b(u,v) = (f,v), \text{ in } \mathcal{D}'(0,T), \tag{5.1}$$

where $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$. Problem (5.1) is completed by the initial condition

$$u(x,0) = u_0(x), \quad \text{in } \Omega. \tag{5.2}$$

The next two theorems show the well-posedness and the regularity of the problem.

the right hand side f is in $L^2(0,T;L^2(\Omega))$, then there exists a unique weak solution u of (5.1), (5.2) in $L^\infty(0,T;L^2(\Omega))\cap L^2(0,T;H^1(\Omega))$.

With the transmission conditions given by $\mathcal{B}_j$ in (3.11), we will need more regularity in our analysis, in the anisotropic Sobolev spaces defined in [20] by

$$H^{r,s}(\Omega\times(0,T)) = L^2(0,T;H^r(\Omega))\cap H^s(0,T;L^2(\Omega)):$$

Theorem 5.2 *Let $\Omega=\mathbb{R}^N$, and m be an integer. If the initial value u_0 is in $H^{2m+1}(\Omega)$, and the right hand side f is in $H^{2m,m}(\Omega\times(0,T))$, then the weak solution u is in $H^{2(m+1),m+1}(\Omega\times(0,T))$.*

For the proofs of Theorems 5.1 and 5.2, and the trace theorems in $H^{r,s}$, we refer to [20].

5.1 Well Posedness of the Algorithm

We first need to study the well-posedness of the subdomain problems with the new boundary conditions. As we saw in the previous section, in order for the convergence factor to be smaller than 1 in modulus, we need $p>0, q\geq 0$. The special case where $q=0$ can be found in [22], and hence, in the sequel, we assume $q\neq 0$. We show here only the analysis for the subproblem on Ω_1, the results for Ω_2 can be found similarly by symmetry. The boundary of Ω_1 is $\Gamma_L=\{L\}\times\mathbb{R}^{N-1}$. Using the boundary operators $\mathcal{S}$ and $\mathcal{B}_1$ defined in (3.11), the problem consists in finding v in an adapted subspace of $\mathcal{C}(0,T;L^2(\Omega_1))\cap L^2(0,T;H^1(\Omega_1))$ such that

$$\begin{aligned} \mathcal{L}v &= f && \text{in } \Omega_1\times(0,T),\\ v(\cdot,0) &= u_0 && \text{in } \Omega_1,\\ \mathcal{B}_1 v &= g_L && \text{on } \Gamma_L\times(0,T). \end{aligned} \tag{5.3}$$

For the variational formulation, we introduce for any real number s the space

$$H^s_s(\Omega_1)=\{v\in H^s(\Omega_1), v_{|\Gamma_L}\in H^s(\Gamma_L)\},$$

where $\cdot_{|\Gamma_L}$ denotes the trace operator on Γ_L. The scalar product in $L^2(\Gamma_L)$ is denoted by $(\cdot,\cdot)_{\Gamma_L}$. The variational formulation is to find $v\in H^1_1$ such that,

$$\begin{aligned} &\forall w\in H^1_1(\Omega_1),\\ &\frac{d}{dt}\big[(v,w)+2q(v,w)_{\Gamma_L}\big]+\frac{1}{2}\big(((\boldsymbol{a}\cdot\boldsymbol{\nabla})v,w)-((\boldsymbol{a}\cdot\boldsymbol{\nabla})v,w)\big)+\nu(\boldsymbol{\nabla}v,\boldsymbol{\nabla}w)+b(v,w)\\ &\qquad+\frac{p}{2}(v,w)_{\Gamma_L}+2q\nu((\boldsymbol{c}\cdot\boldsymbol{\nabla_y})v,w)_{\Gamma_L}+2q\nu^2(\boldsymbol{\nabla_y}v,\boldsymbol{\nabla_y}w)_{\Gamma_L}=(f,v),\ \text{in } \mathcal{D}'(0,T). \end{aligned}$$

Theorem 5.3 *For $p>0$ and $q>0$, if f is in $L^2(0,T,L^2(\Omega_1))$, u_0 is in $H^1_1(\Omega_1)$, and g_L is in $L^2((0,T)\times\Gamma_L)$, then the subdomain problem (5.3) has a unique solution v in $L^2(0,T,H^2_2(\Omega_1))\cap H^1(0,T;H^0_0(\Omega_1))$.*

Proof The proof is based on *a priori* estimates: multiplying equation (5.3) by v and integrating in space, and then using the boundary condition, we obtain

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\left[\|v(\cdot,t)\|^2_{L^2(\Omega_1)}+2q\|v(\cdot,t)\|^2_{L^2(\Gamma_L)}\right]+\nu\|\boldsymbol{\nabla}v(\cdot,t)\|^2_{L^2(\Omega_1)}+b\|v(\cdot,t)\|^2_{L^2(\Omega_1)}\\ &+\frac{p}{2}\|v(\cdot,t)\|^2_{L^2(\Gamma_L)}+2q\nu^2\|\boldsymbol{\nabla_y}v(\cdot,t)\|^2_{L^2(\Gamma_L)}=(f(\cdot,t),v(\cdot,t))+\nu(g(\cdot,t),v(\cdot,t))_{\Gamma_L}. \end{aligned}$$

On the right-hand side we use the Cauchy-Schwarz inequality together with the inequality

$$\alpha\beta\leq\frac{\eta}{2}\,\alpha^2+\frac{1}{2\eta}\,\beta^2,\quad \text{for all } \alpha,\beta\in\mathbb{R}, \text{ and } \eta>0. \tag{5.4}$$

If $b=0$, we need furthermore the Gronwall Lemma. We obtain by integration in time a bound for v, with a constant C depending on the physical constants b,ν, the parameters p and q, and the length of the time interval T:

$$\|v\|^2_{L^\infty(0,T,H^0_0(\Omega_1))}+\|v\|^2_{L^2(0,T;H^1_1(\Omega_1))}\leq C(\|f\|^2_{L^2(0,T,L^2(\Omega_1))}+\|g\|^2_{L^2(0,T,L^2(\Gamma_L))}). \tag{5.5}$$

condition to obtain

$$\frac{1}{2}\frac{d}{dt}\left[b\|v(\cdot,t)\|^2_{L^2(\Omega_1)}+\nu\|\boldsymbol{\nabla} v(\cdot,t)\|^2_{L^2(\Omega_1)}+\frac{p-a}{2}\|v(\cdot,t)\|^2_{L^2(\Gamma_L)}+q\nu^2\|\boldsymbol{\nabla_y} v(\cdot,t)\|^2_{L^2(\Gamma)}\right]$$
$$+\|\partial_t v(\cdot,t)\|^2_{L^2(\Omega_1)}+2q\|\partial_t v(\cdot,t)\|^2_{L^2(\Gamma_L)}$$
$$=(f(\cdot,t),\partial_t v(\cdot,t))+(g(\cdot,t),\partial_t v(\cdot,t))_{\Gamma_L}-((\boldsymbol{a}\cdot\boldsymbol{\nabla})v(\cdot,t),\partial_t v(\cdot,t))+2q\nu((\boldsymbol{c}\cdot\boldsymbol{\nabla_y})v(\cdot,t),\partial_t v(\cdot,t))_{\Gamma_L}.$$

Using the Cauchy-Schwarz inequality together with (5.4) as before, integrating in time and using (5.5), we obtain

$$\|v\|^2_{L^\infty(0,T,H^1_1(\Omega_1))}+\|\partial_t v\|^2_{L^2(0,T;H^0_0(\Omega_1))}\le C'(\|f\|^2_{L^2(0,T,L^2(\Omega_1))}+\|g\|^2_{L^2(0,T,L^2(\Gamma_L))}),$$

where the constant C' depends also on $\boldsymbol{a}$. We complete the result by using the equation, which gives

$$\Delta v\in L^2(0,T;L^2(\Omega_1)),\quad \partial_x v-2q\nu\Delta_{\boldsymbol{y}} v\in L^2(0,T;L^2(\Gamma_L)).$$

A regularity theorem proved in [29] asserts that this implies $v\in L^2(0,T;H^2_2(\Omega_1))$, and gives a bound for the norm in $L^2(0,T;H^2_2(\Omega_1))$. Now we have altogether a bound for v in $L^2(0,T,H^2_2)\cap H^1(0,T;H^0_0(\Omega_1))$. This first proves uniqueness. Using a Galerkin method, we obtain the existence result. ∎

The previous result suffices to define the algorithm in the non-overlapping case. The overlapping case however requires more regularity.

Theorem 5.4 *For $p>0$ and $q>0$, let f be in $H^{2,1}(\Omega_1\times(0,T))$, u_0 be in $H^3(\Omega)$, and g_L be in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))$, with the compatibility condition*

$$g_L(\cdot,0)=\partial_x u_0(L,\cdot)+\frac{p-a}{2\nu}u_0(L,\cdot)+2q(\nu\partial_{xx}u_0(L,\cdot)-a\partial_x u_0(L,\cdot)-bu_0(L,\cdot)+f(L,\cdot,0)). \tag{5.6}$$

Then the solution v of the subdomain problem (5.3) is in $H^{4,2}(\Omega_1\times(0,T))$. Furthermore, the following compatibility property at $x=0$ is satisfied:

$$\lim_{t\to0+}\mathcal{B}_2 v(0,\cdot,t)=\partial_x u_0(0,\cdot)-\frac{p+a}{2\nu}u_0(0,\cdot)-2q(\nu\partial_{xx}u_0(0,\cdot)-a\partial_x u_0(0,\cdot)-bu_0(0,\cdot)+f(0,\cdot,0)).$$

Proof With the assumptions in the Theorem, the solution u of (3.1) is indeed in $H^{4,2}(\Omega_1\times(0,T))$ by Theorem 5.2, and by the Trace Theorem in [20], $\tilde g_L=\mathcal{B}_1 u(L,\cdot,\cdot)$ is in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))$, and satisfies the compatibility condition (5.6). Defining $h=g_L-\tilde g_L$, $e=v-u$ is the solution of

$$\begin{array}{rcll}\mathcal{L}e&=&0&\text{in }\Omega_1\times(0,T),\\ e(\cdot,0)&=&0&\text{in }\Omega_1,\\ \mathcal{B}_1 e&=&h&\text{on }\Gamma_L\times(0,T).\end{array}\tag{5.7}$$

Since h is in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))$, and $h(\cdot,0)=0$, we can extend it in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times\mathbb{R})$ by $\tilde h$ vanishing on $\Gamma\times\mathbb{R}_-$. Then we extend in time the first equation and the boundary condition in (5.7) to $\Gamma_L\times\mathbb{R}$. The solution $\tilde e$ of the extended problem is an extension of e. We finally Fourier transform the resulting equation in time and $\boldsymbol{y}$. By (3.4), the Fourier transform of e is given in terms of $\mathcal{F}\tilde h$, the Fourier transform of $\tilde h$, by

$$\mathcal{F}\tilde e(\boldsymbol{\eta},\omega)=\frac{2\nu}{f(z)+s(z)}\mathcal{F}\tilde h(\boldsymbol{\eta},\omega)e^{\frac{a+f(z)}{2\nu}(x-L)},\tag{5.8}$$

with $z=i(\omega+\boldsymbol{c}\cdot\boldsymbol{\eta})+\nu|\boldsymbol{\eta}|^2$. We introduce $\tau=\omega+\boldsymbol{c}\cdot\boldsymbol{\eta}$. With the definition of f, and using that $p>0$, $q>0$, we obtain

Lemma 5.1 *There exist positive constants D,D' such that*

$$\frac{2\nu}{|f(z)+s(z)|}\le D(\tau^2+|\boldsymbol{\eta}|^4)^{-1/2},\quad \frac{\nu}{a+\Re f(z)}\le D'(\tau^2+|\boldsymbol{\eta}|^4)^{-1/4},\quad |r^+|^2\sim 2(\tau^2+|\boldsymbol{\eta}|^4)^{1/2}.$$

For large τ and $\boldsymbol{\eta}$, we have

$$|r^+|^2\sim 2(\tau^2+|\boldsymbol{\eta}|^4)^{1/2}.$$

$$\|\partial_t^2\tilde e\|^2_{L^2(\Omega_1\times\mathbb{R})} = \int_{-\infty}^{L}\int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}} \frac{4\nu^2\omega^4}{\left|f(z)+s(z)\right|^2}\ |\mathcal{F}\tilde h(\boldsymbol{\eta},\omega)|^2 e^{2\Re r^+(x-L)}dx\,d\boldsymbol{\eta}\,d\omega,$$

or after integration in the x variable,

$$\|\partial_t^2\tilde e\|^2_{L^2(\Omega_1\times\mathbb{R})} = \int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}} \frac{4\nu^2\omega^4}{\left|f(z)+s(z)\right|^2}\ \frac{\nu}{a+\Re f(z)}|\mathcal{F}\tilde h(\boldsymbol{\eta},\omega)|^2 d\boldsymbol{\eta}\,d\omega.$$

We have by Lemma 5.1, for large τ and $\boldsymbol{\eta}$,

$$\frac{4\nu^2\omega^4}{\left|f(z)+s(z)\right|^2}\ \frac{\nu}{a+\Re f(z)} \le D^2D'(\tau-\boldsymbol{c}\cdot\boldsymbol{\eta})^4(\tau^2+|\boldsymbol{\eta}|^4)^{5/4} = D^2D'\frac{(\tau-\boldsymbol{c}\cdot\boldsymbol{\eta})^4}{(\tau^2+|\boldsymbol{\eta}|^4)^2}(\tau^2+|\boldsymbol{\eta}|^4)^{3/4}.$$

Since $\tilde h$ is in $H^{\frac32,\frac34}(\Gamma_L\times\mathbb{R})$, we obtain

$$\|\partial_t^2\tilde e\|^2_{L^2(\Omega_1\times\mathbb{R}^2)} \le D''\|\tilde h\|^2_{H^{\frac32,\frac34}(\Gamma_L\times\mathbb{R})}.$$

For the spatial derivatives, we proceed as before, and we have for $j+k\le 4$,

$$\|\partial_x^k\partial_{y_l}^j\tilde e\|^2_{L^2(\Omega_1\times\mathbb{R})} = \int_{\mathbb{R}^{n-1}\times\mathbb{R}} \frac{4\nu^2 r_+^{2k}\eta_l^{2j}}{\left|f(z)+s(z)\right|^2}\ \frac{\nu}{a+\Re f(z)}|\mathcal{F}\tilde h(\omega)|^2 d\boldsymbol{\eta}\,d\omega.$$

From the bound on the integrand for large τ and $\boldsymbol{\eta}$,

$$\frac{4\nu^2 r_+^{2k}\eta_l^{2j}}{\left|f(z)+s(z)\right|^2}\ \frac{\nu}{a+\Re f(z)} \le D^2D'2^k(\tau^2+|\boldsymbol{\eta}|^4)^{(k+j)/2},$$

we conclude as before that all space derivatives up to order 4 are square integrable, and finally we have

$$\|\tilde e\|_{H^{4,2}(\Omega_1\times\mathbb{R})} \le \bar D\|\tilde h\|_{H^{\frac32,\frac34}(\Gamma_L\times\mathbb{R})}.$$

Taking the infimum over all extensions $\tilde h$ gives

$$\|e\|_{H^{4,2}(\Omega_1\times(0,T))} \le C\|h\|_{H^{\frac32,\frac34}(\Gamma_L\times(0,T))}.$$

Similarly, we see that

$$\|\mathcal{S}\tilde e(0,\cdot,\cdot)\|^2_{H^{\frac32,\frac34}(\Gamma_L\times\mathbb{R}))} = \int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}} \frac{4\nu^2|z|^2}{\left|f(z)+s(z)\right|^2}(1+\omega^2)^{\frac32}\ (1+|\boldsymbol{\eta}|^2)^3\ |\mathcal{F}\tilde h(\omega)|^2 e^{-2\Re r^+L}d\boldsymbol{\eta}\,d\omega,$$

and therefore $\mathcal{S}e(0,\cdot)$ is in $H^{\frac32,\frac34}(\Gamma_L\times(0,T))$, with

$$\|\mathcal{S}e\|^2_{H^{\frac32,\frac34}(\Gamma_L\times(0,T))} \le Ce^{-\frac{aL}{\nu}}\|h\|_{H^{\frac32,\frac34}(\Gamma_L\times(0,T))}.$$

For the compatibility property, since $\tilde h$ is supported in $\Gamma_L\times\mathbb{R}_+$, $\mathcal{F}\tilde h$ is analytic in the half-plane $\Im\omega<0$, and by (5.8) and the Paley-Wiener Theorem [26], $\tilde e(0,\cdot,\cdot)$ is supported in $\Gamma_L\times\mathbb{R}_+$ as well. Since e is in $H^{4,2}(\Omega_1\times(0,T))$, $\partial_x e$ is in $H^{\frac52,\frac54}(\Gamma_L\times(0,T))$, and hence all quantities in $\mathcal{B}_2e$ are continuous on $[0,T]$, and therefore $\lim_{t\to0_+}\mathcal{B}_2e(0,\cdot,t)=0$, which completes the proof of the theorem. ■

We are now ready to show the well posedness of the algorithm: let g_L be given on Γ_L and let g_0 be given on $\Gamma_0=\{0\}\times\mathbb{R}^{N-1}$, and let $p>0$ and $q>0$. We define for $k=1,2,\dots$ the iterations by algorithm (3.2), initialized by

$$\mathcal{B}_1u_1^1=g_L \ \text{ on } \Gamma_L\times(0,T),\quad \mathcal{B}_2u_2^1=g_0 \ \text{ on } \Gamma_0\times(0,T), \tag{5.9}$$

Consider first the nonoverlapping case: $L=0$. Then it is easy to obtain:

$k = 1, 2, \ldots$, *the algorithm* (3.2) *with the transmission operators given in (3.11), initialized with (5.9) defines a unique sequence of iterates* (u_1^k, u_2^k) *in* $L^2(0,T,H_2^2(\Omega_1)) \cap H^1(0,T;H_0^0(\Omega_1)) \times L^2(0,T,H_2^2(\Omega_2)) \cap H^1(0,T;H_0^0(\Omega_2))$.

In the overlapping case, we need to use the compatibility condition in Theorem 5.4:

Theorem 5.6 *Let* $L > 0$, $p > 0$ *and* $q > 0$, f *be in* $H^{2,1}(\Omega_1 \times (0,T))$, u_0 *be in* $H^3(\Omega)$, g_L *and* g_0 *be given in* $H^{\frac{3}{2},\frac{3}{4}}(\mathbb{R}^{n-1} \times (0,T))$, *with the compatibility conditions*

$$g_L(\cdot,0) = \partial_x u_0(L,\cdot) + \frac{p-a}{2\nu} u_0(L,\cdot) + 2q(\nu\partial_{xx}u_0(L,\cdot) - a\partial_x u_0(L,\cdot) - bu_0(L,\cdot) + f(L,\cdot,0)),$$
$$g_0(\cdot,0) = \partial_x u_0(0,\cdot) - \frac{p+a}{2\nu} u_0(0,\cdot) - 2q(\nu\partial_{xx}u_0(0,\cdot) - a\partial_x u_0(0,\cdot) - bu_0(0,\cdot) + f(0,\cdot,0)).$$

Then, for $k = 1, 2, \ldots$, *the algorithm* (3.2) *with the transmission operators given in (3.11), initialized by (5.9) defines a unique sequence of iterates* (u_1^k, u_2^k) *in* $H^{4,2}(\Omega_1 \times (0,T)) \times H^{4,2}(\Omega_2 \times (0,T))$.

5.2 Convergence of the Algorithm

Theorem 5.7 *For* $p > 0$ *and* $q > 0$, *under the conditions of existence of the algorithm, the sequence* (u_1^k, u_2^k) *converges to* $(u_{|\Omega_1}, u_{|\Omega_2})$.

Proof We return to the analysis in Section 3, which has been validated by the previous theorems. The Fourier transforms in time and $\boldsymbol{y}$ of the errors satisfy

$$\hat{e}_1^{2k+1}(x,\boldsymbol{\eta},\omega) = \rho^k \hat{e}_1^1(x,\boldsymbol{\eta},\omega), \quad \hat{e}_1^{2k}(x,\boldsymbol{\eta},\omega) = \rho^{k-1}\hat{e}_2^1(x,\boldsymbol{\eta},\omega),$$
$$\hat{e}_2^{2k+1}(x,\boldsymbol{\eta},\omega) = \rho^k \hat{e}_2^1(x,\boldsymbol{\eta},\omega), \quad \hat{e}_2^{2k}(x,\boldsymbol{\eta},\omega) = \rho^{k-1}\hat{e}_1^1(x,\boldsymbol{\eta},\omega).$$

For p and q strictly positive, we have $|\rho| < 1$ for all $(\omega, \boldsymbol{\eta})$ in $(\mathbb{R} \times \mathbb{R}^{n-1})$. By the Lebesgue Theorem, we conclude the proof. ■

Remark 5.1 *The results in this Section generalize the analysis from [22] to the case when the operator* S *contains the transverse Laplace operator* Δ_y. *In [22], the proof of convergence in the non-overlapping case is based on clever energy estimates, and as such extends to variable coefficients.*

6 Numerical Results

We perform in this section one-dimensional numerical experiments to measure the convergence factors of the numerical implementation of the various Schwarz waveform relaxation algorithms analyzed at the continuous level in this paper. We use the parabolic model problem (3.1) on the domain $\Omega = (0,6)$. We impose homogeneous boundary conditions, $u(0,t) = 0$ and $u(6,t) = 0$, and use various initial conditions $u(x,0)$, $x \in \Omega$.

6.1 Experiments with Two Subdomains

We first use a decomposition of the domain Ω into the two subdomains $\Omega_1 = (0, L_2)$ and $\Omega_2 = (L_1, 6)$, $L_1 \le L_2$, and hence $L = L_2 - L_1$. We refer with the term iteration to a double iteration of the respective algorithms, since for two subdomains, one can perform all the iterations in an alternating fashion and thus obtain the even iterates on one subdomain and the odd ones on the other, without having to compute the remaining ones. We show only results of numerical experiments for the algorithm with overlap, since with overlap, we can compare the results to the classical Schwarz waveform relaxation algorithm with Dirichlet transmission conditions, which does not converge without overlap. We chose for the problem parameters $\nu = 0.2$, $a = 1$, $b = 0$. We discretize (3.1) using an upwind finite difference discretization in space with mesh parameter $\Delta x = 0.02$, and a backward Euler discretization in time, with time step $\Delta t = 0.005$. We chose $L_1 = 2.96$ and $L_2 = 3.04$, which means the overlap is $L = 0.08$, and we compute the numerical solution in the time interval $[0, T = 2.5]$. Using as initial condition

$$u(x,0) = e^{-3(1.2-x)^2},$$

$T = 2.5$, where we started the algorithm with a zero initial guess, both for the classical and the optimized waveform relaxation algorithm. In Figure 5 on the left,

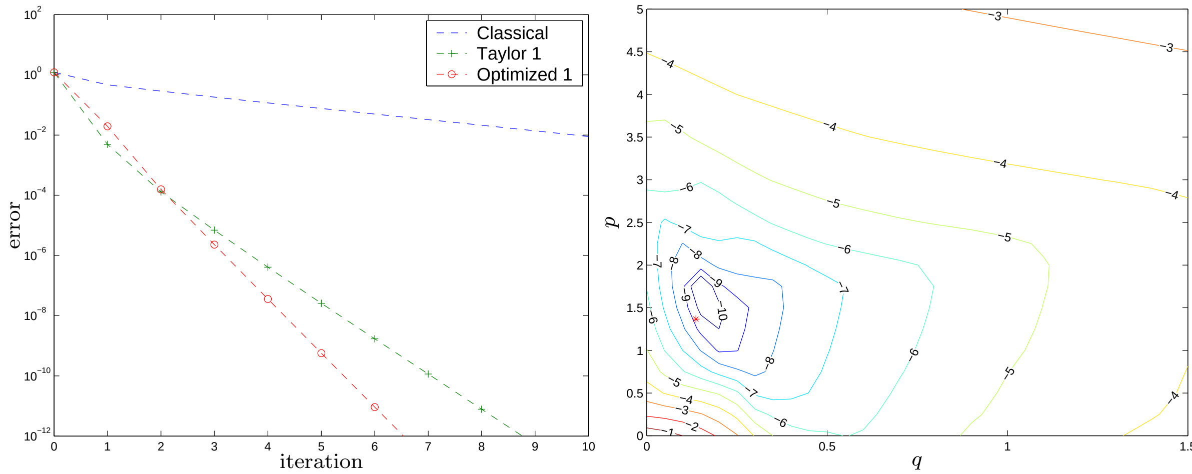

Figure 5: **Left:** convergence factors of the classical Schwarz waveform relaxation algorithm with Dirichlet transmission conditions compared to the same algorithm with the new first order transmission conditions. **Right:** the error obtained running the algorithm with first order transmission conditions for 5 steps and various choices of the free parameters p and q, and indicated by a star the choice p^*, q^* predicted by the theory.

one can see the performance of the classical algorithm and the one with first order Taylor conditions, $p = p_T = 1$ and $q = q_T = 0.4$, and with optimized parameters, which were found to be $p = p^* = 1.366061845$ and $q = q^* = 0.1363805228$ using Theorem 4.3. It is important to realize that the computational cost per iteration of all these algorithms is the same: a change in the transmission conditions does not affect the local solver cost on each subdomain.

In Figure 5 on the right, we performed five iterations of the optimized Schwarz waveform relaxation algorithm with first order transmission conditions, varying the free parameters p and q, and show the base 10 logarithm of the error obtained. We indicate by a star the optimal parameters p^*, q^* predicted by Theorem 4.3. This shows that the continuous analysis predicts the optimal choice very well.

To illustrate the asymptotic results given in Theorem 4.3 for the Taylor conditions and in Theorem 4.4 for the optimized ones, we choose the same problem parameters as before, but start now with a coarser mesh both in space and time, $\Delta x = 0.04$ and $\Delta t = 0.01$, and we fix the overlap to be $L = \Delta x$. We then run the optimized Schwarz waveform Relaxation algorithm with first order Taylor and optimized transmission conditions until the error becomes smaller than 10^{-14}, and count the number of iterations. We repeat this experiment dividing Δx and Δt by 2 several times. This corresponds for the first order Taylor conditions to the case in Theorem 4.3 where the convergence factor should behave like $1 - O(\sqrt{\Delta x})$, and for the first order optimized conditions to the case in Theorem 4.4 where the convergence factor should behave like $1 - O(\Delta x^{\frac{1}{8}})$, almost independent of Δx. Figure 6 shows on the left

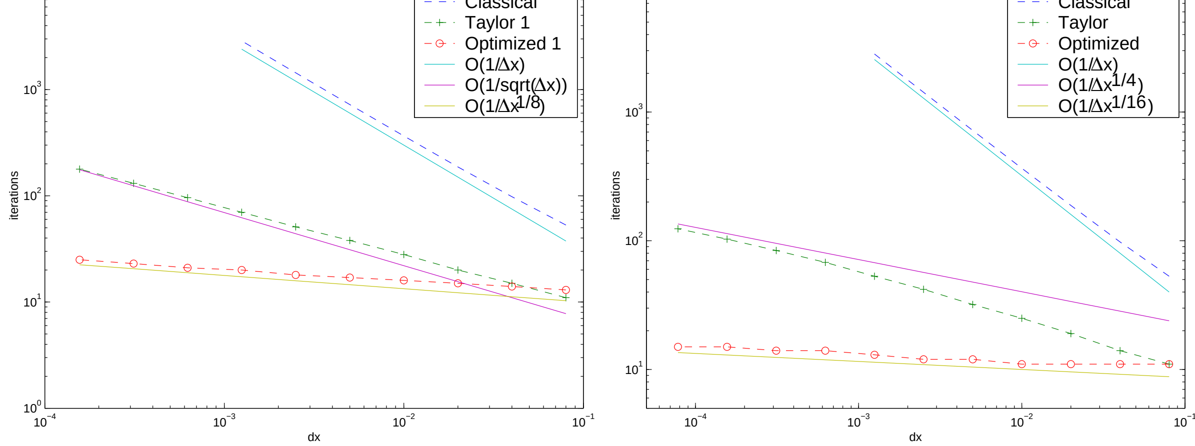

Figure 6: Asymptotic behavior as the mesh is refined with an overlap $L = \Delta x$: on the left the case where $\Delta t = O(\Delta x)$ and on the right where $\Delta t = O(\sqrt{\Delta x})$, together with the predicted rates from the analysis, both for the classical and the optimized Schwarz waveform relaxation algorithms with Taylor and optimized first order transmission conditions.

the results obtained from these experiments. One can see that the asymptotic analysis predicts very well the numerical behavior of the algorithms. Next, we perform a similar experiment, starting with the same values for Δx and Δt, but now we divide Δx by 2 each time and Δt only by $\sqrt{2}$ (such a refinement is admissible, since our scheme is implicit), which implies $\Delta t = O(\sqrt{\Delta x})$. While this does not change anything for the classical algorithm, which still has the same bad convergence factor $1 - O(\Delta x)$, for the algorithm with Taylor first order transmission conditions now case 3 of Theorem 4.3 applies, and the algorithm should show the much better convergence factor $1 - O(\Delta x^{\frac{1}{4}})$. The optimized Algorithm has according to Theorem 4.4 now the even better convergence factor $1 - O(\Delta x^{\frac{1}{16}})$, virtually independent of Δx. In Figure 6 on the right, one can clearly see that this is the case. The algorithm has different asymptotic convergence factors with the same overlap, depending on the discretization in time, as predicted.

6.2 Experiments with Eight Subdomains

We now show experiments which indicate that the results we obtained for two subdomains are also relevant for many subdomains. Using the same model problem as before, we now decompose the domain into eight subdomains. In Figure 7, we show in the top row the first 3 iterations of the classical Schwarz waveform relaxation algorithm, and below the same iterations for the algorithm with optimized first order transmission conditions.

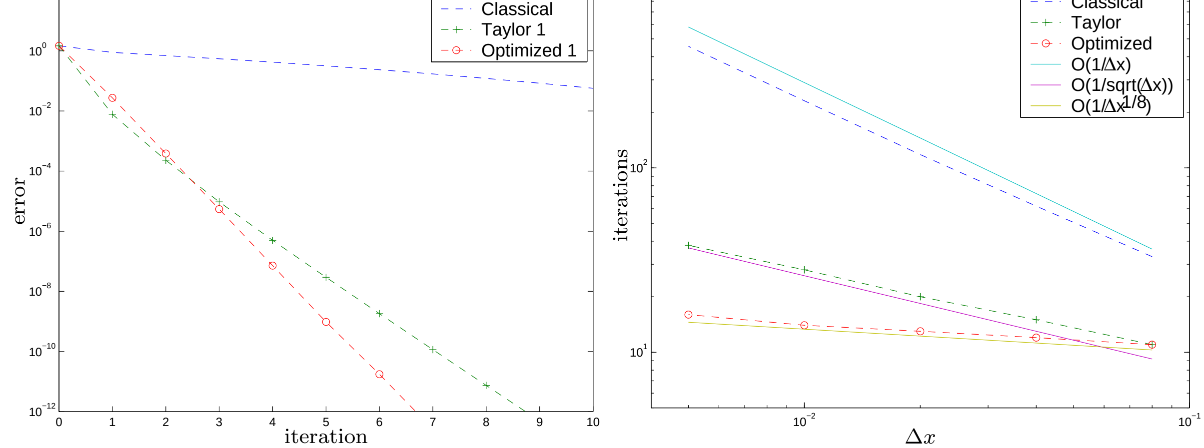

Figure 8: **Left:** convergence factor comparison for the eight subdomain case. **Right:** Asymptotic behavior as the mesh is refined with an overlap $L = \Delta x$ for the eight subdomain case, with $\Delta t = O(\Delta x)$, together with the predicted rates from the two subdomain analysis.

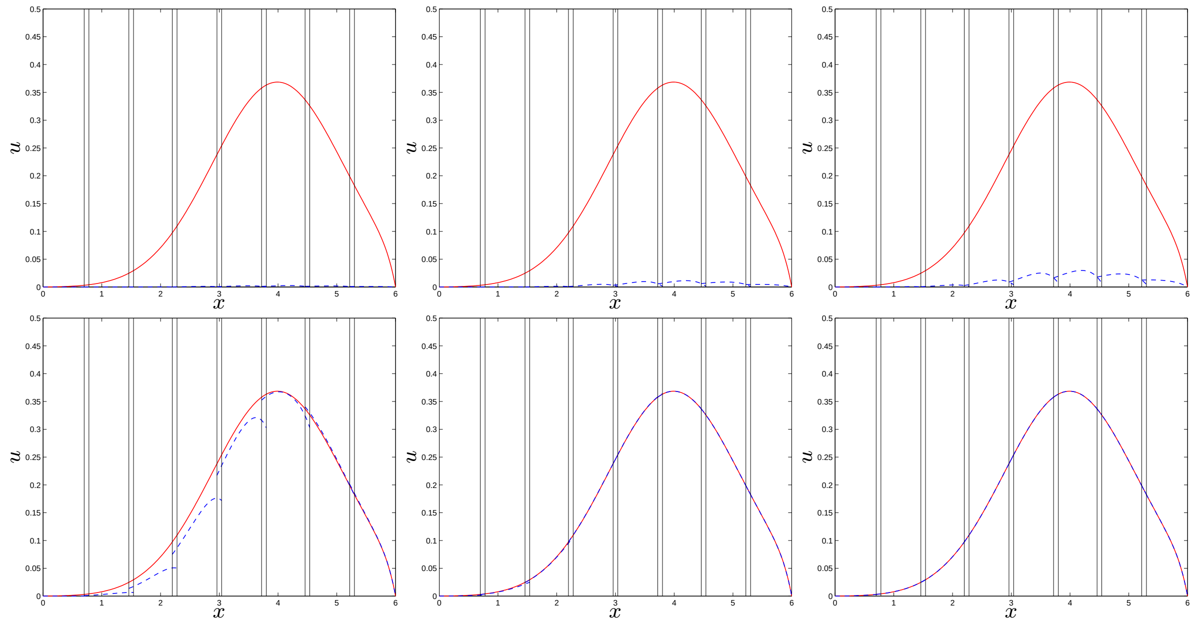

Figure 7: From left to right, the first, second and third iterates $u_j^k(x,T)$, $j = 1,\ldots,8$ (dashed) at the end of the time interval $t = T$ together with the exact solution (solid) for the same model problem as before: top row the classical and bottom row the optimized algorithm.

This clearly shows how important the transmission conditions are in the many subdomain case. We show the corresponding convergence factors in Figure 8 on the left, and on the right we perform the same asymptotic experiments as in Figure 6 on the left, but now with eight subdomains, which indicates that the results of Theorems 4.3 and 4.4 also hold for more than two subdomains.

7 Conclusions

We presented and analyzed a homographic best approximation problem for complex functions of one complex variable, which is important for the performance of a new class of waveform relaxation algorithms. We showed that the best approximation problem has at least one solution and that all solutions satisfy an equioscillation property. In the case of a compact domain, we also proved that the solution is

waveform relaxation algorithm, whose performance relies on the optimization of the convergence factor on a range of relevant discrete frequencies. Using the general results in the first part, we were able to prove an "overequioscillation property" for this particular problem, which leads to explicit formulae for the optimal parameters in one dimension. We also derived asymptotic formulas, both for the one and higher dimensional cases, which permit the direct use of the optimized algorithms in practice.
We showed that the new algorithm is well posed and convergent, and that it greatly outperforms the classical one. Our analyses concern both the overlapping and nonoverlapping cases. Therefore the new algorithm can be used with or without overlap, which is an advantage for local adaptation in space-time. Further improvements of our work will concern higher dimensions with variable coefficients.

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